声子晶体能带结构的数值计算方法及带隙调控

汪越胜

北京交通大学

国家自然科学基金重点项目

国家留学基金委-德国DAAD联合PPP项目

内容

一）从固体能带理论说起

二）什么是声子晶体（弹性波带隙材料）

三）独特的声学特征—带隙

四）广阔的应用前景

五）带隙调控—带隙工程

六）声学特性的表征参量

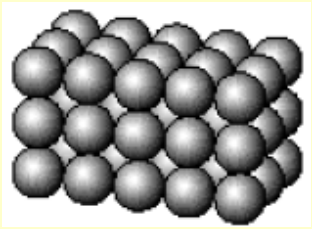
八）能带结构的数值计算方法

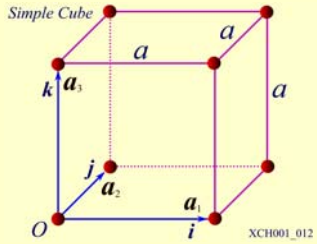
九）展望

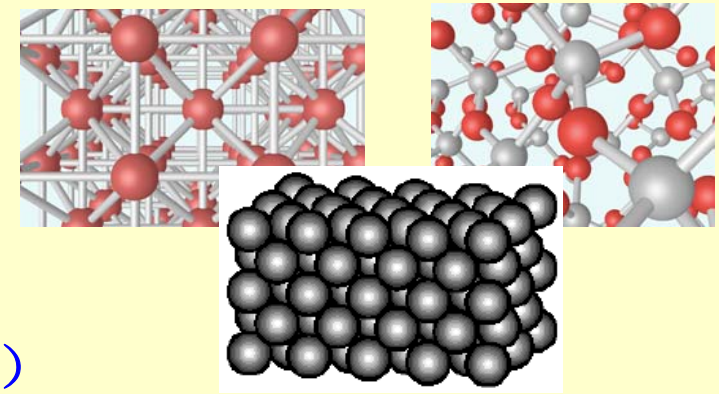
从固体能带理论说起-1

——关于固体输运性质最成功的（近似）理论

晶体







晶格---原子排列方式（⇔点阵、**Bravais**格子）

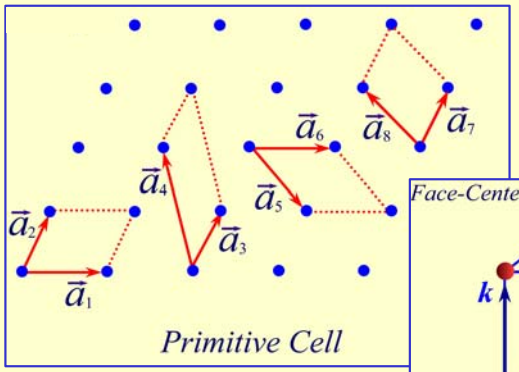
原胞—最小周期单元（⇔单胞）

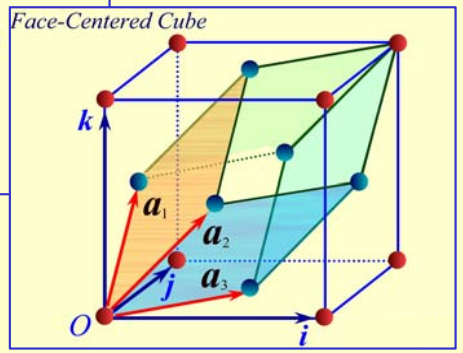
格矢： $\mathbf{R} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3$

$\mathbf{a}_1\ \mathbf{a}_2\ \mathbf{a}_3$ --- 基矢

$l_1\ l_2\ l_3$ --- 格点，整数

$\mathbf{r} = \mathbf{r}_a + \mathbf{R}$





从固体能带理论说起-2

物理量在空间的周期性： $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$ $\Rightarrow$ **Fourier级数**

倒格子和倒格矢： $\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

$\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ --- 倒格子基矢，[长度]$^{-1}$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

$$V_{\mathbf{G}} = \frac{1}{\Omega_0}\iiint_{\Omega_0} V(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}$$

倒格原胞：。。。

从固体能带理论说起-3

单电子运动（近似）

Schrödinger 方程(定态):

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r})$$

Bloch波(定理):

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$ 平面波

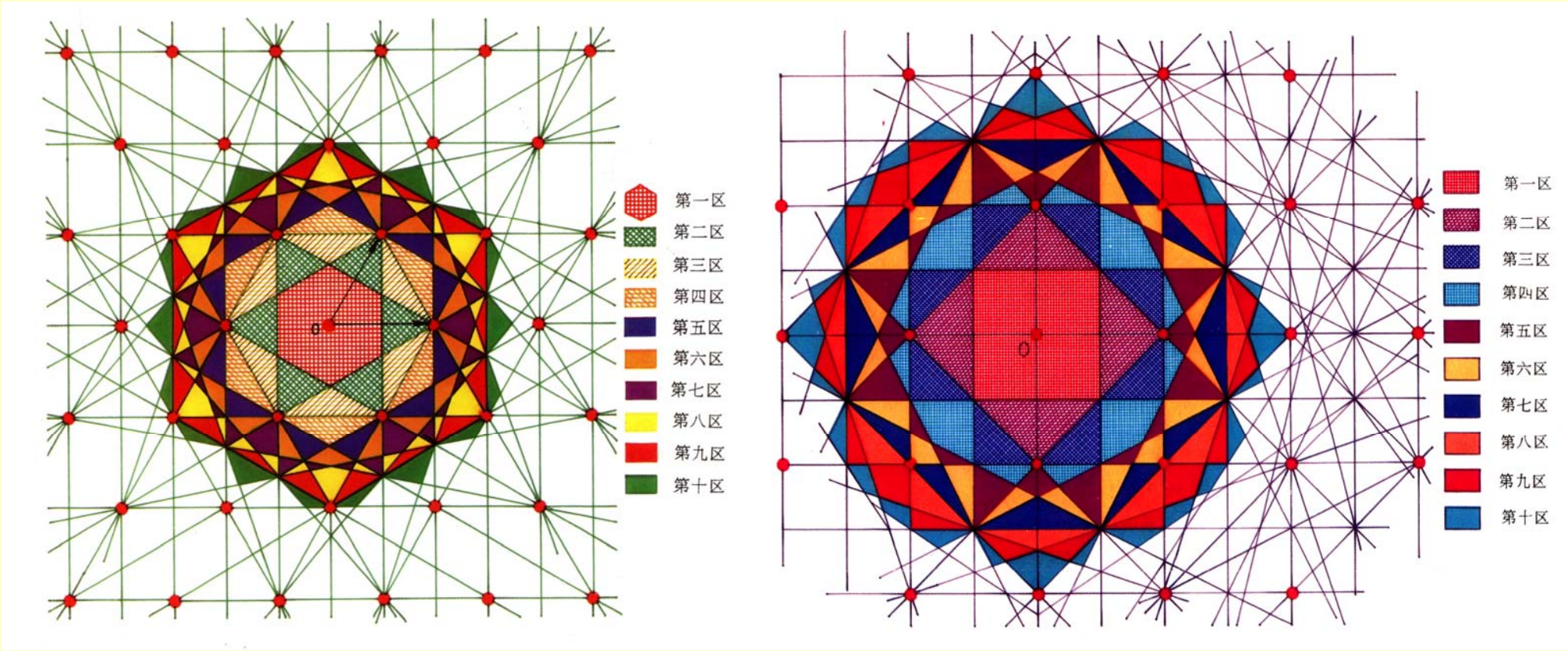
$$u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$$

$$\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\psi_{\mathbf{k}} = \psi_{\mathbf{k}+\mathbf{G}}$$ **(k态≡k+G态)**

从固体能带理论说起-4

Brillouin区（第一～，简约～）： 由从原点出发的倒格矢的垂直平分面所围的区域



从固体能带理论说起-5

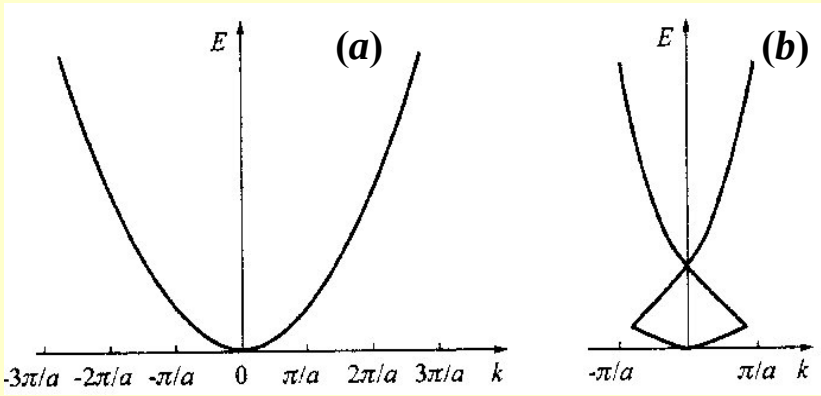
自由电子气模型：

$$V(\mathbf{r}) = 0$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \Omega^{-1/2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$E(\mathbf{k}) = \hbar^2 k^2 / 2m$$

频(色)散关系

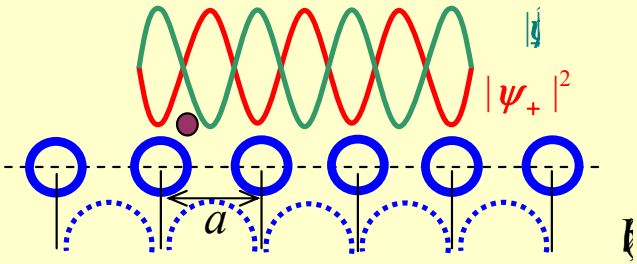


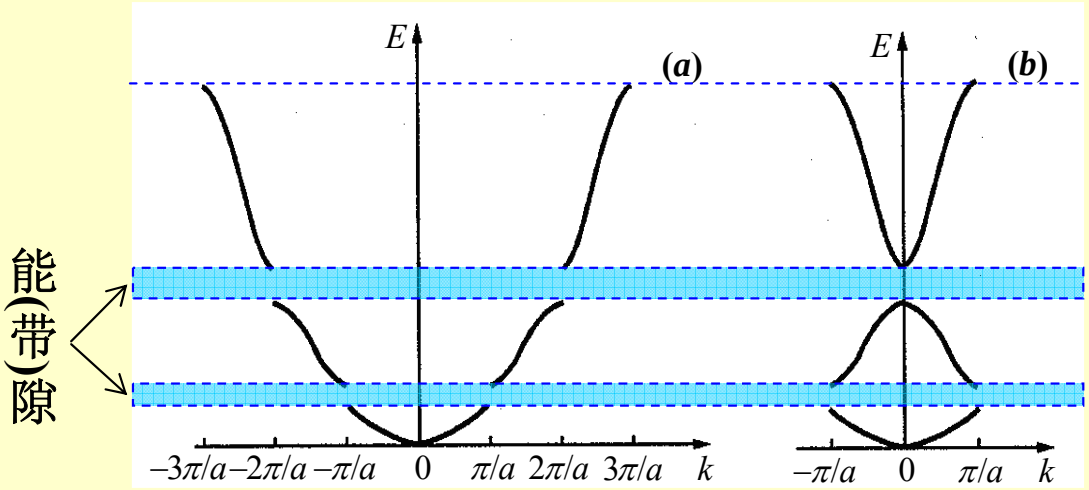
一维自由电子模型的能带(连续)
(a)扩展区方案；(b) 简约区方案

连续的频散关系！

从固体能带理论说起-6

近自由电子模型：





一维近自由电子模型的能带和带隙
(a)扩展区方案；（b）简约区方案

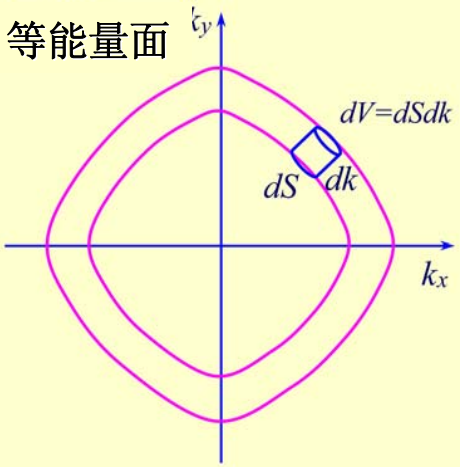
当电子波矢k落在Brillouin区界面上时，即当波矢为k的Bloch波波长满足Bragg条件时，波将受到晶格的全反射，反射波与入射波幅值相等，引起波的相消干涉，形成驻波，从而使能谱中出现禁带，即产生带隙，将能谱分裂成能带。所以电子能隙的出现与电子波的Bragg散射直接相关。

从固体能带理论说起-7

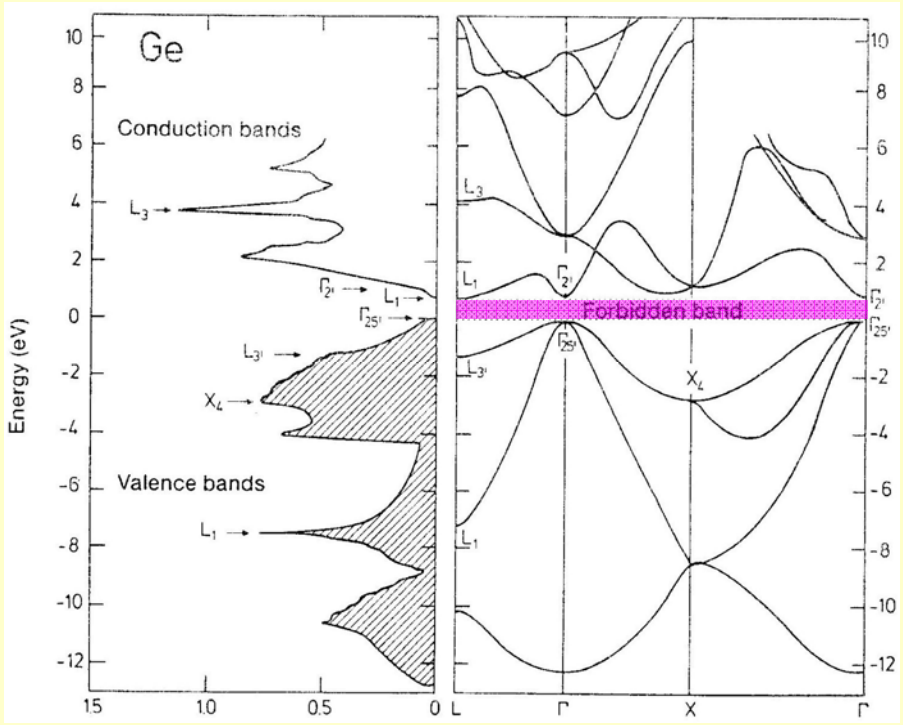
三维情况

态密度(DOS)：单位体积和单位能量间隔($E\sim E+\Delta E$)内态的数目(ΔZ)

态密度函数：$$N(E)=\lim\frac{\Delta Z}{\Delta E}$$

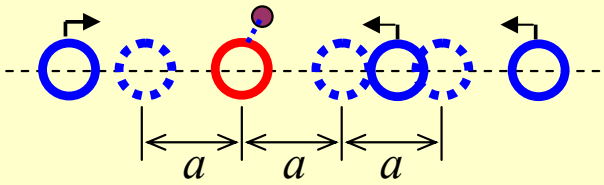


$$N(E)=\frac{\Omega}{(2\pi)^3}\int\frac{dS}{|\nabla_k E|}$$



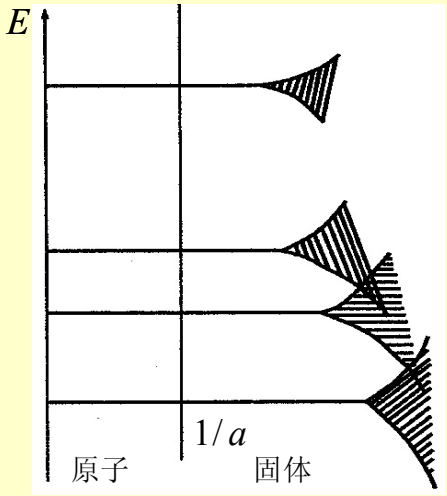
态密度(DOS)　　能带(出现交叠)

紧束缚电子模型：



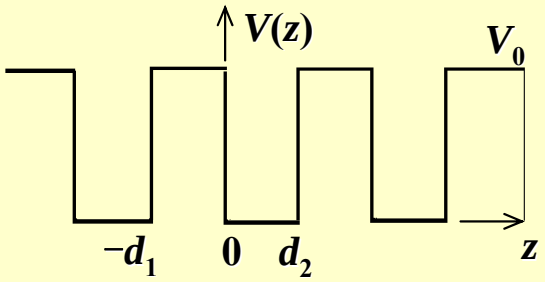
当原子相互接近组成晶体时，原子之间的相互作用增强，原来孤立的每一能级扩展为能带，且随着原子间距减小而增宽。若能带宽度的增加没有淹没最初两个电子态之间的能级差，就产生能隙。

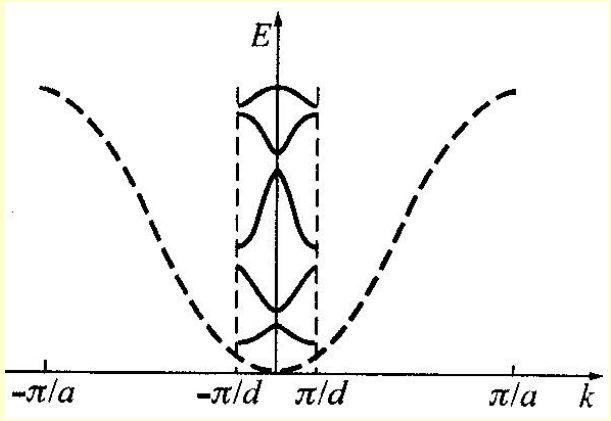
能带和能隙就像是离散电子态之间的能级差在晶体情况下遗留的痕迹，因而能隙的存在主要取决于原子局域的电子态，对结构的周期性没有严格要求。这说明，结构的周期性对称不再是能隙存在的必要条件。



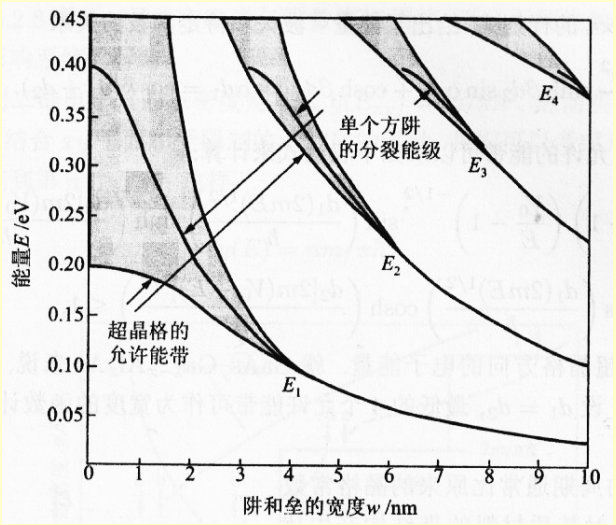
紧束缚电子模型的原子能级扩展为能带

超晶格(Kronig-Penney模型):





$d\ (=d_1+d_2) > a$



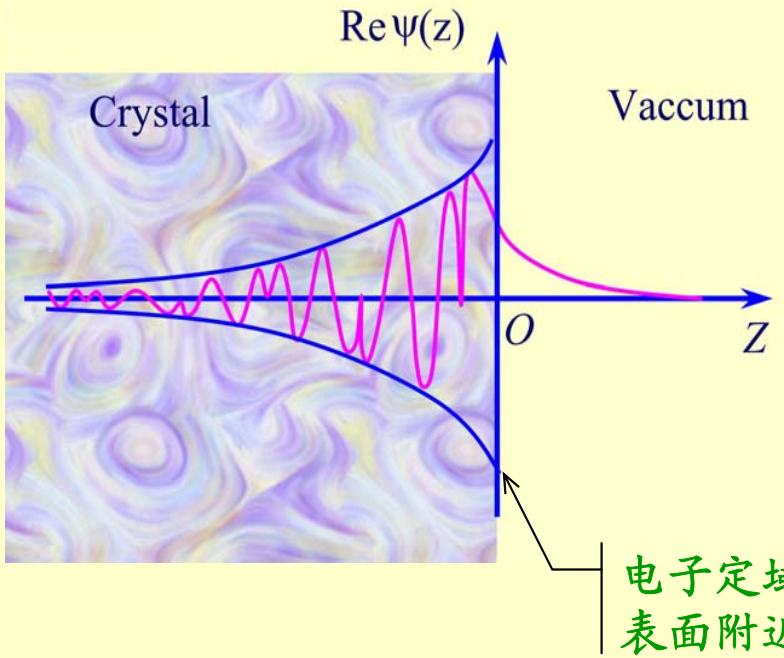
GaAs-$Ga_{1-x}Al_xAs$

局(定)域态----表面态和杂质态：

表面----对周期性的破坏

1D： $\psi_k(\mathbf{r}) = A\mathrm{e}^{\mathrm{i}kz}$

Im(k)=0时，扩展态；
Im(k)>0时，局域态(表面态)

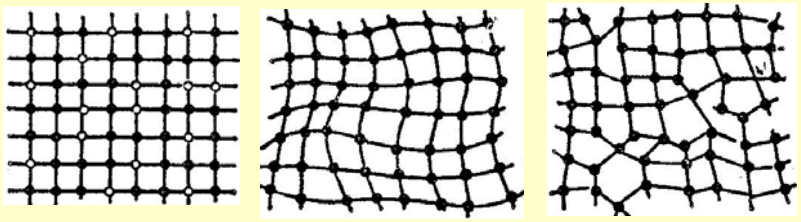


3D： $\psi_{\mathbf{k}}(\mathbf{x},z) = A_{\mathbf{k}}(\mathbf{x})\mathrm{e}^{\mathrm{i}\mathbf{k}_{//}\cdot\mathbf{x}}\mathrm{e}^{\mathrm{i}k_z z}$

Im($k_{//}$)=0时，x-y平面内扩展态；
Im(k_z)>0时，z方向局域态(表面态)

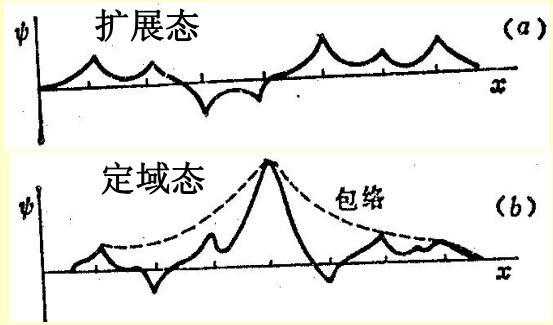
杂质----对周期性的破坏----局域态(杂质态)

从固体能带理论说起-12



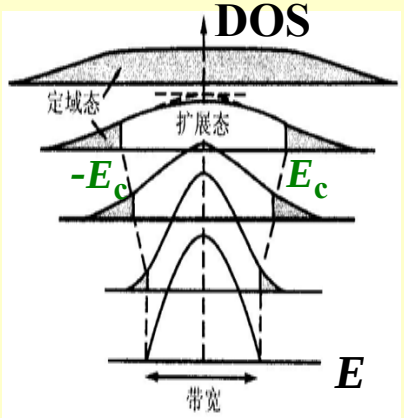
无序----Anderson局域化：

不再是Bloch波，$E(k)$不再适用，可用态密度。



无序程度比较小时，部分定域态和部分扩展态；
无序程度足够大时，全部为定域态。

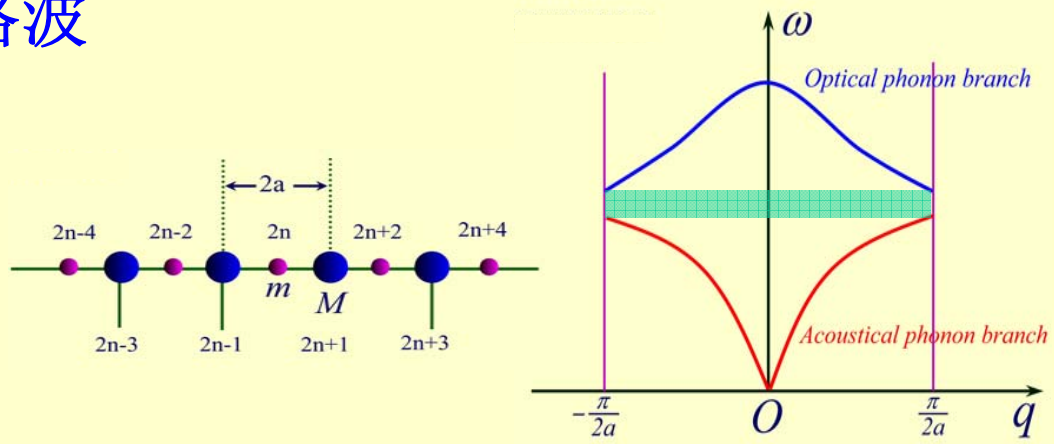
参杂⇒无序度⇒金属-绝缘体转变⇒参杂半导体(Mott)
(Anderson转变)

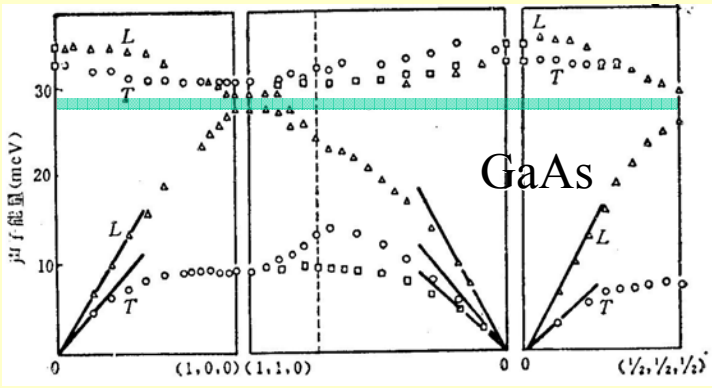


准周期（短程无序、长程有序，周期 <*> 无序）

扩展态 < 临界态 > 定域态

格波





光波（电磁波）⇒ 光子晶体（1987）

声波（弹性波）??? （1993，Kushwaha, et.al.）

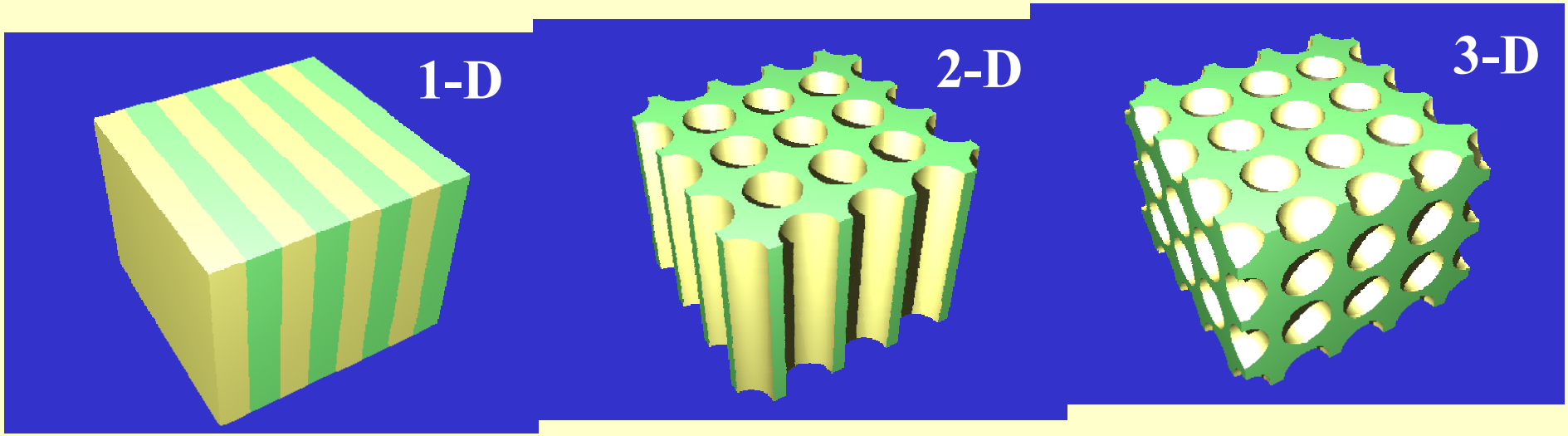
声子晶体—弹性波带隙材料

具有能带结构(分离的色散关系，弹性波禁带)

一定频率范围内声波不能透过介质传播(无声子态)

一种周期复合介质

(1维、2维、3维；固-固、固-液、固-气)



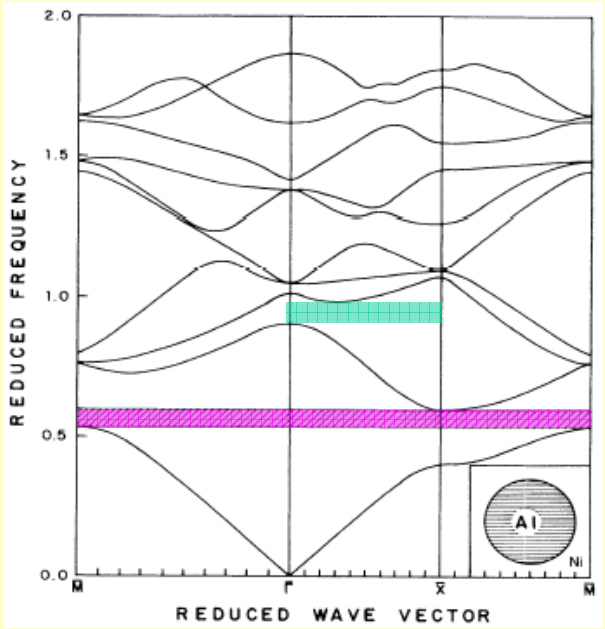
声子晶体—光子晶体—电子（晶体）

属性	晶体		光子晶体	声子晶体
介质构成	结晶体 （自然的或生长的）		两种或以上介电材料 组成的复合介质	两种或以上弹性材料 组成的复合介质
参量	普适常数，原子数	原子质量，力常数， 原子数	各组元的介电常数	各组元的质量密度和弹 性模量（或声波波速）
晶格常数	1～5Å （微观）		0.1μm~1cm （介观或宏观）	介观或宏观
波的形式	de Broglie 波 （电子）ψ	格波 （声子）$\mathbf{u}$	电磁波或光波 （光子）$\mathbf{E}$, $\mathbf{B}$	弹性波 （声子）$\mathbf{u}$
偏振	纵波	横波和纵波	横波	横波和纵波 （$\nabla\times\mathbf{U}\neq 0$）
波动方程	$-\frac{\hbar^2}{2m}\nabla^2\psi+V(\mathbf{r})\psi$ $=i\hbar\frac{\partial}{\partial t}\psi$	$-\sum_{ls'j}\Phi_{ls,ls'j}u_{ls'j}$ $=M_s\frac{\partial^2 u_{ls}}{\partial t^2}$	$\nabla^2\mathbf{E}-\nabla(\nabla\cdot\mathbf{E})$ $=\frac{\varepsilon(\mathbf{r})}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2}$	弹性波动方程 $[\mu(\mathbf{r})(u_{i,j}+u_{j,i})]_{,j}+$ $[\lambda(\mathbf{r})u_{j,j}]_{,i}=\rho(\mathbf{r})\frac{\partial^2 u_i}{\partial t^2}$
自有粒子 极限	$W=\frac{\hbar^2k^2}{2m}$ （电子）	$\omega=ck$ （声子）	$\omega=\frac{c}{\sqrt{\varepsilon}}k$ （光子）	$\omega=ck$ （声子）
带隙	随晶格势增加而增 大，无电子态存在	随原子质量差$\lvert M_a-M_b\rvert$ 的增加而增大， 无声子态存在	随介电常数差$\lvert\varepsilon_a-\varepsilon_b\rvert$ 的增加而增大， 无光子态存在	随质量密度差$\lvert\rho_a-\rho_b\rvert$ 的增加而增大， 无声子态存在
频率范围	无线电波、微波、 光波和 X 射线	$\omega>1$ GHz （低频率时采用连续介质 的弹性波近似）	微波、光波	$\omega\leq 1$ GHz

波传播现象的统一性

声学特征——带隙：产生机理

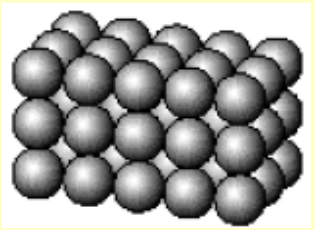
Bragg散射机理



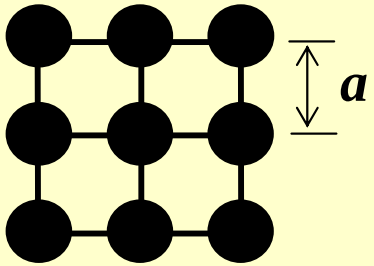
方向带隙

完全带隙

Kushwaha, et.al. PRL, 1993
（铝/镍）



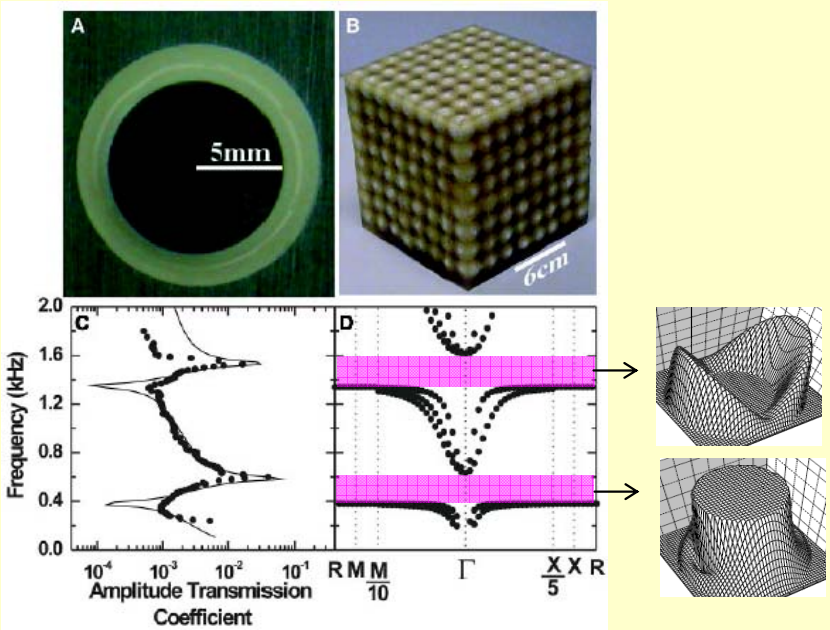
晶体中电子波的**Bragg**散射



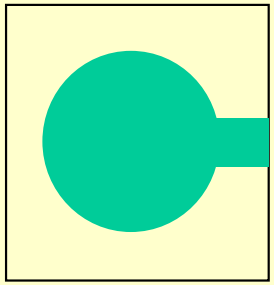
严格周期性要求
依赖于晶格尺寸(与波长同量级)

声学特征——带隙：产生机理

局域共振机理



Liu, et.al. Science, 2000
（橡胶涂层铅球/环氧）



Helmholz 共振腔

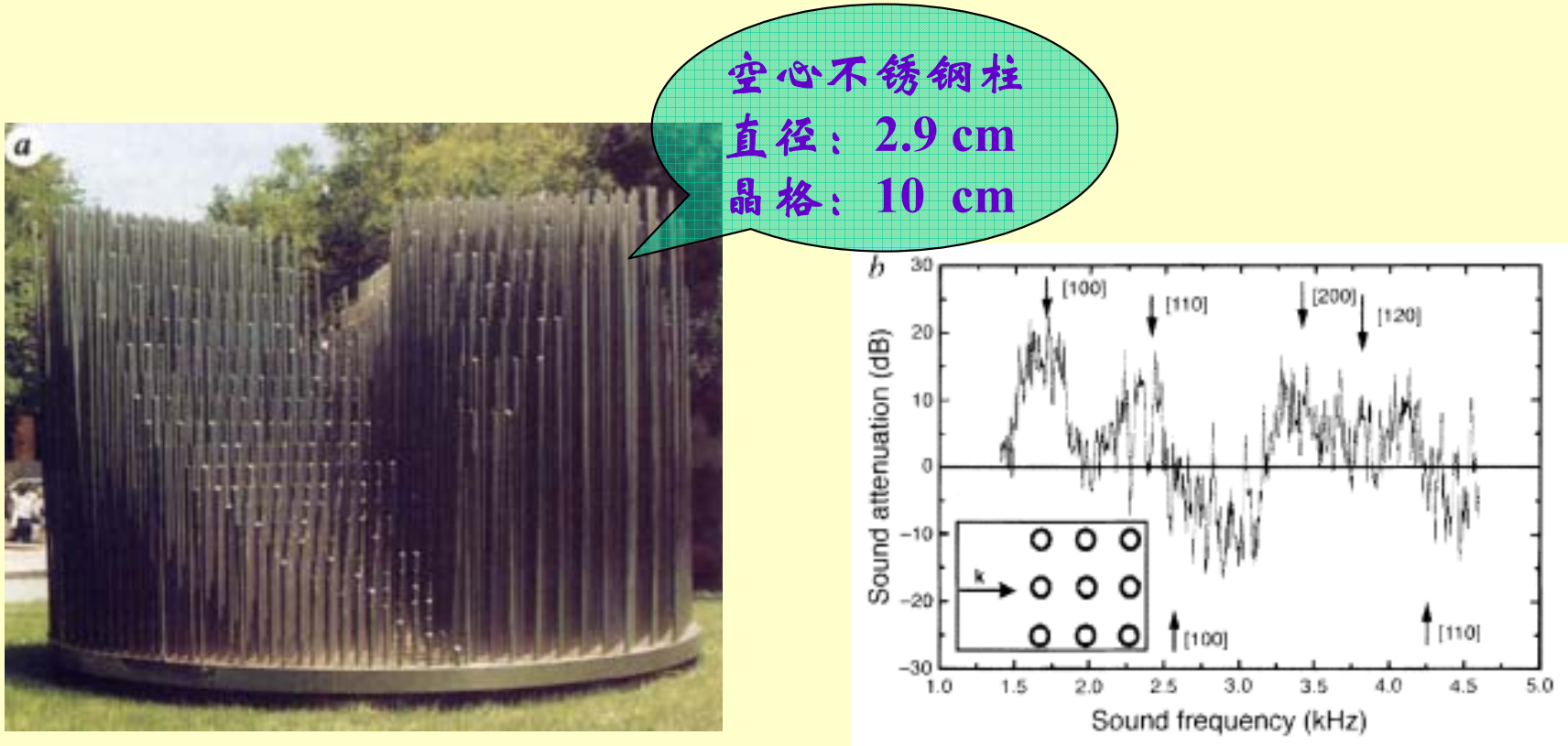
紧束缚电子模型

取决于单元的振动特性
波长>>晶格尺寸

声学特征——带隙：产生机理

一个有趣的声子晶体实例：

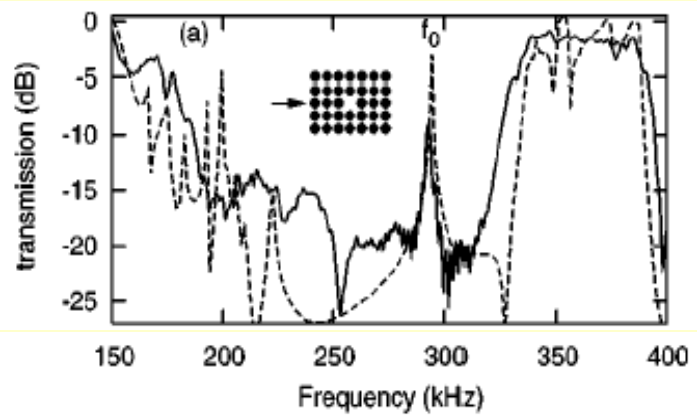
西班牙马德里某广场上的雕塑 ——运动的旋律

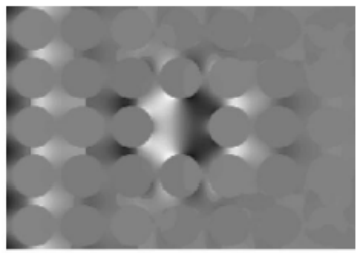


Martinez-Sala et al. Nature, 1995.

声学特征—带隙及缺陷态

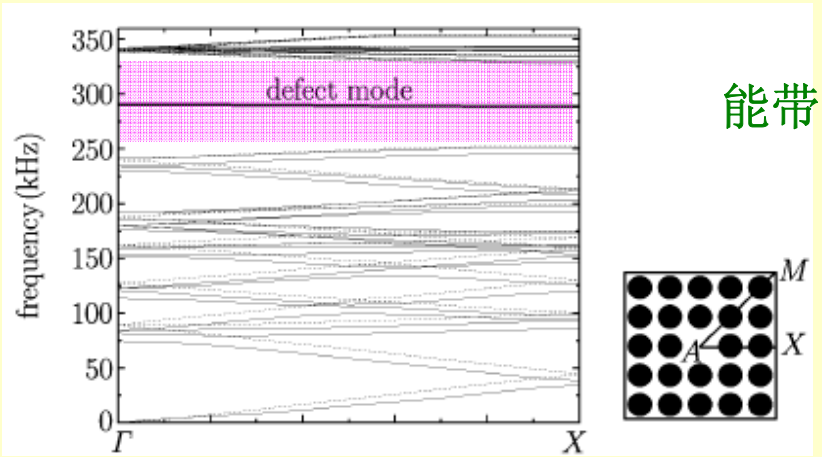
点缺陷，波局域化



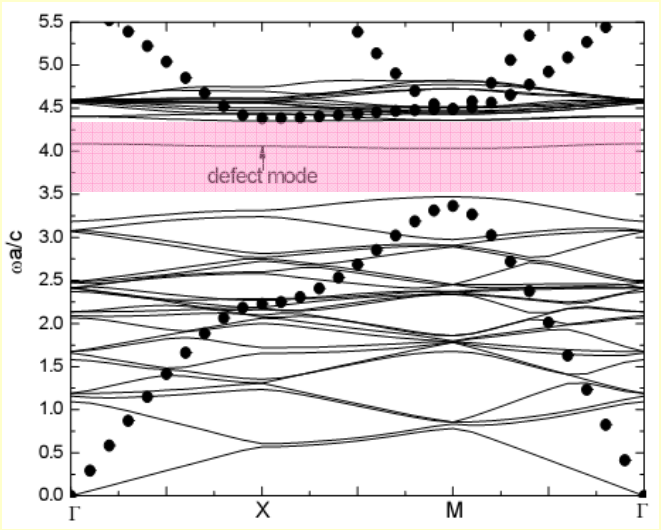


响应谱

Khelif, et. al. PRB, 2003
(Steel/Water)



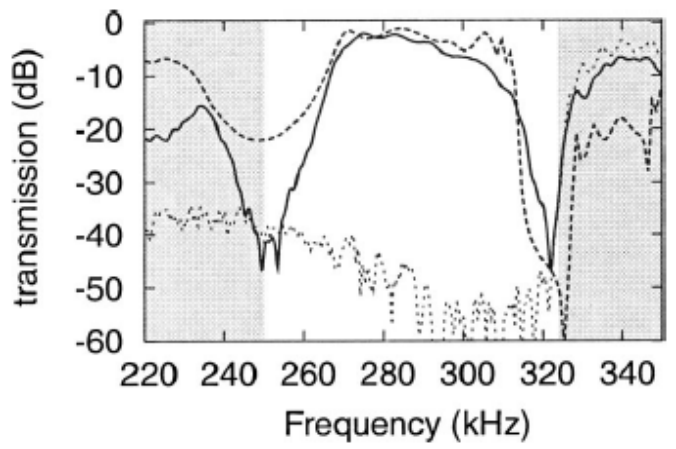
能带结构



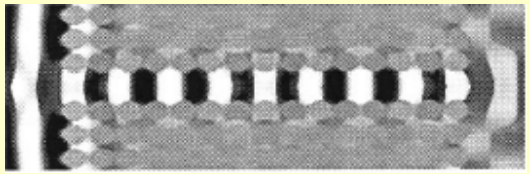
Yan, et. al. AMSS, 2008

声学特征——带隙及缺陷态

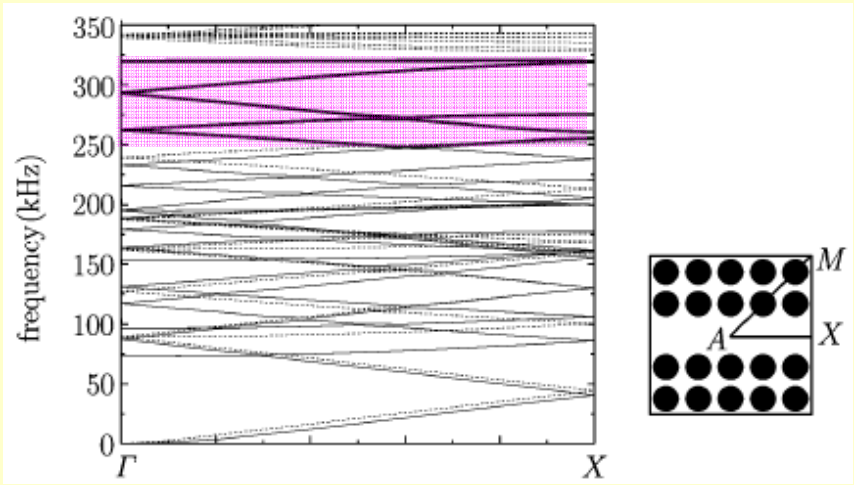
线缺陷，波局域化



响应谱



Khelif, et. al. APL, 2004
(Steel/Water)



能带结构

Yan, et. al. AMSS, 2008

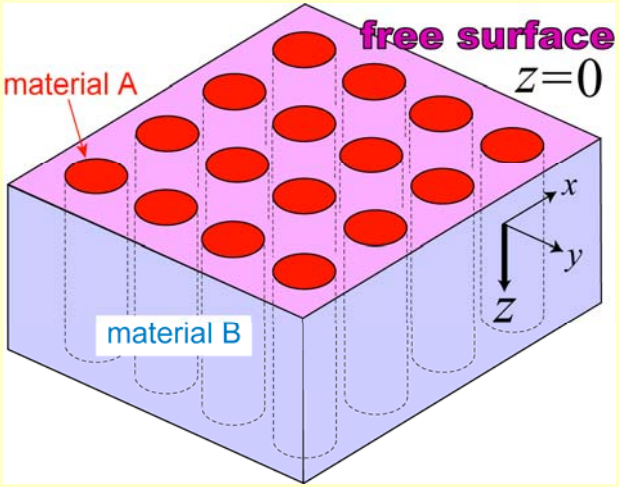
声学特征—表面态带隙

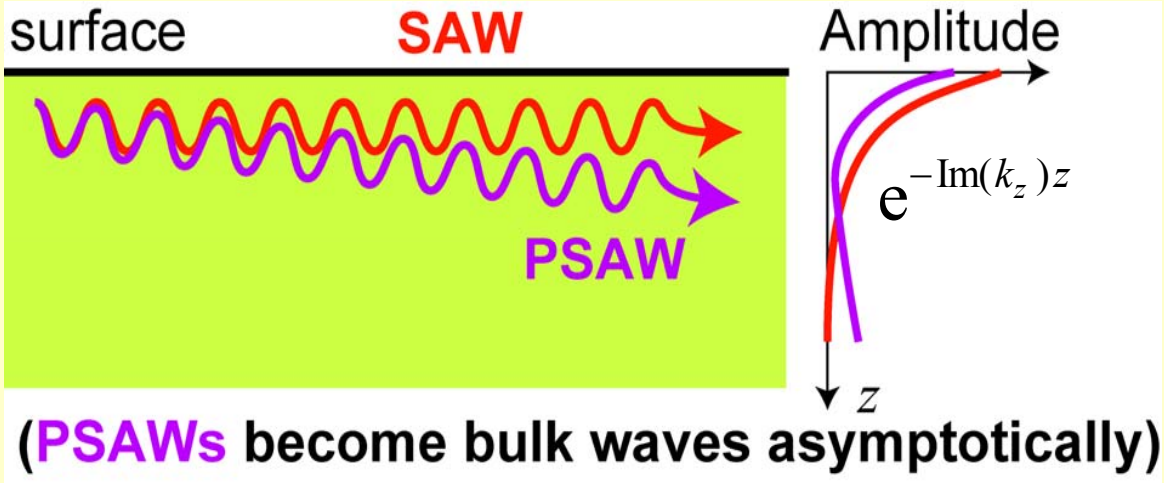
表面波模态

$$\mathbf{u}(\mathbf{r},t)=\mathrm{e}^{\mathrm{i}(\mathbf{k}_{//}\cdot\mathbf{x}-\omega t)}\mathrm{e}^{\mathrm{i}k_z z}\sum_{\mathbf{G}}\mathbf{u}_{\mathbf{k}}(\mathbf{G})\mathrm{e}^{\mathrm{i}\mathbf{G}\cdot\mathbf{x}}$$

$\mathbf{k}_{//}$ – **real number** $(\mathrm{Im}\,k_z>0)$ **：表面波(SAW)**

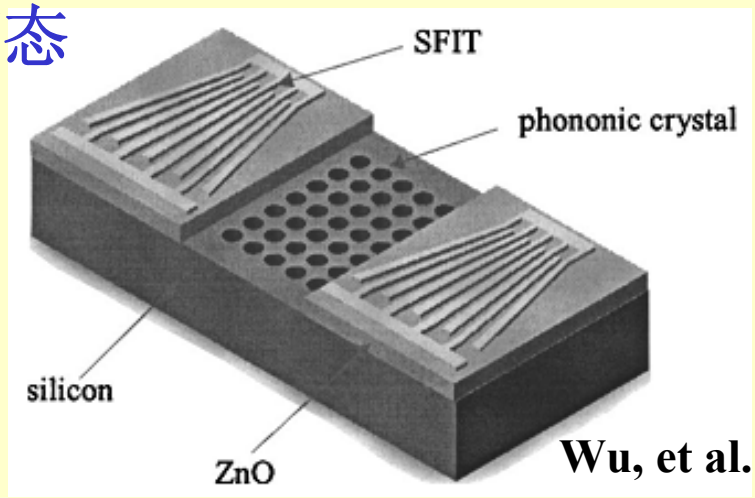
$\mathbf{k}_{//}\Rightarrow\mathbf{k}_{//}(1+\mathrm{i}\varepsilon)$ $(\mathrm{Im}\,k_z<0)$**：伪表面波(PSAW)**





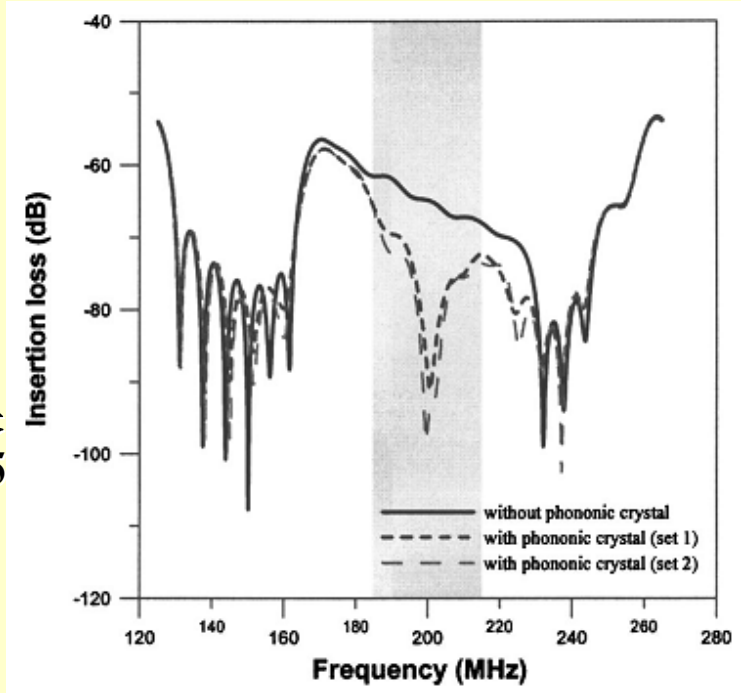
声学特征—表面态带隙

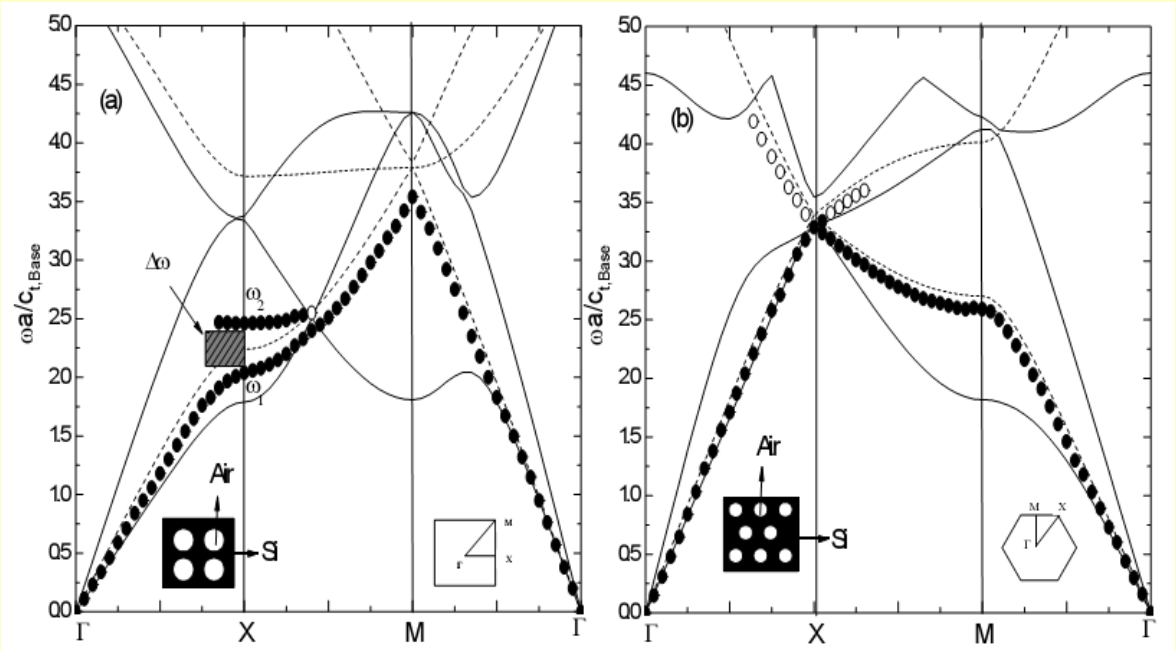
表面波模态



测试结果

Wu, et al. JAP, 2005





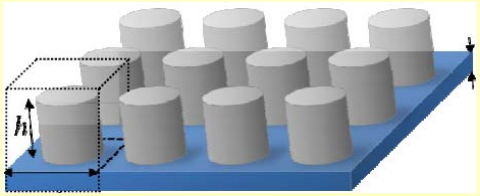
空气/硅

小波计算结果

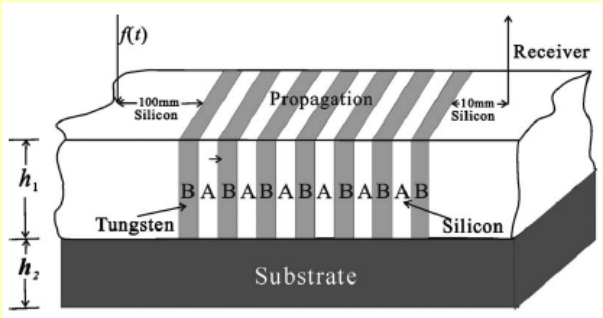
Yan, Wang, PRB, 2008

声学特征—板波带隙

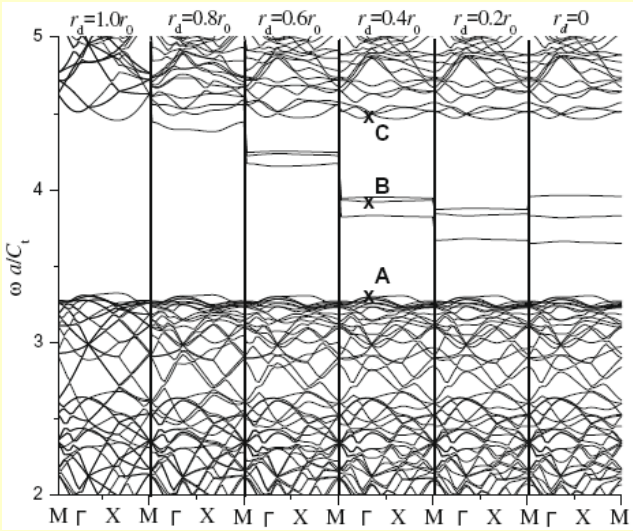
板中的Lamb波和弯曲波



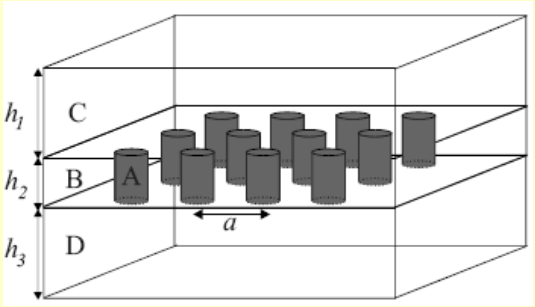
Pennec, et al. PRB, 2008



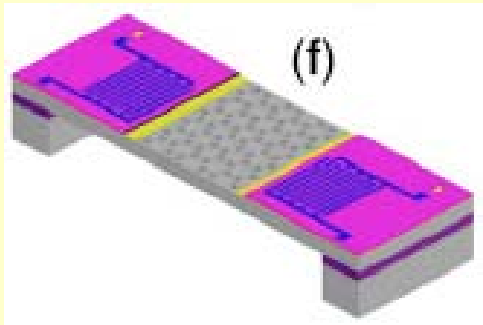
Gao, et al. APL, 2008



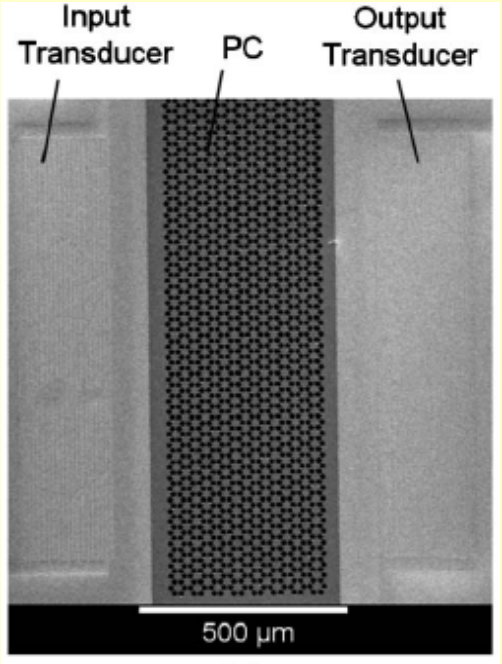
Yao, Yu, Wang, et al. IJSS, 2009

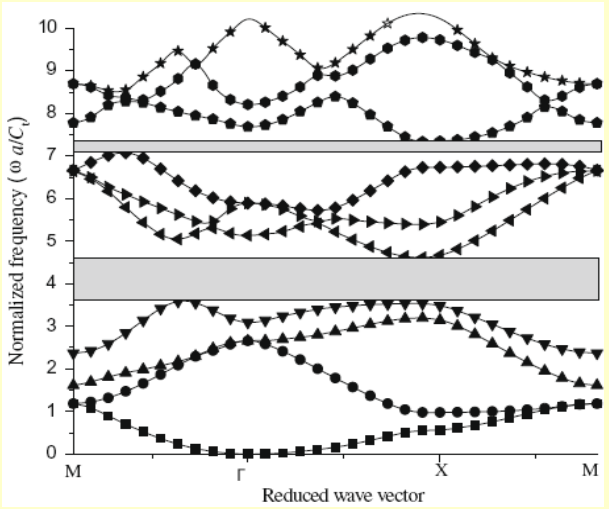


Vasseur, et al. PRB, 2008



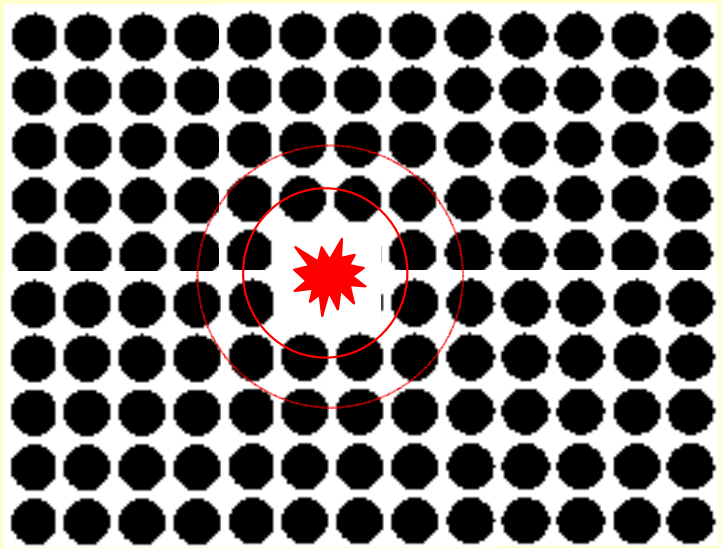
Mohammadi, et al. APL, 2008

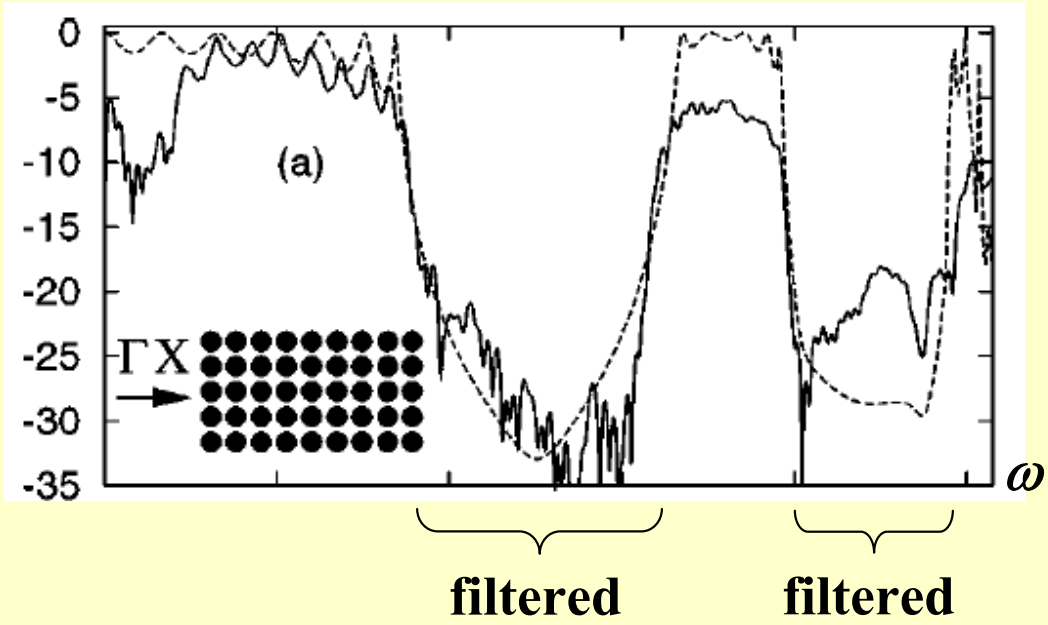




广阔的应用前景-1

带隙 ⇔ 隔音降噪，声滤波器

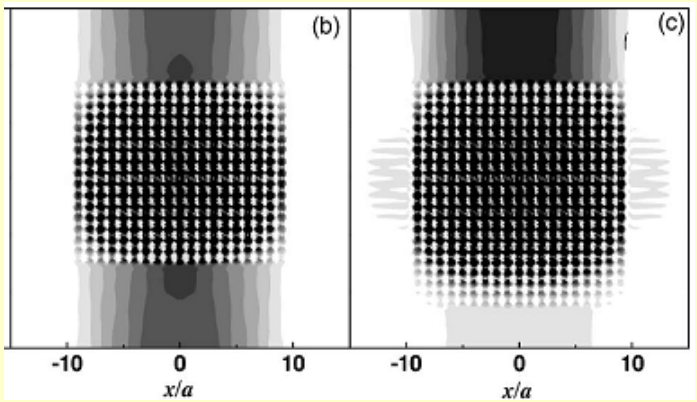




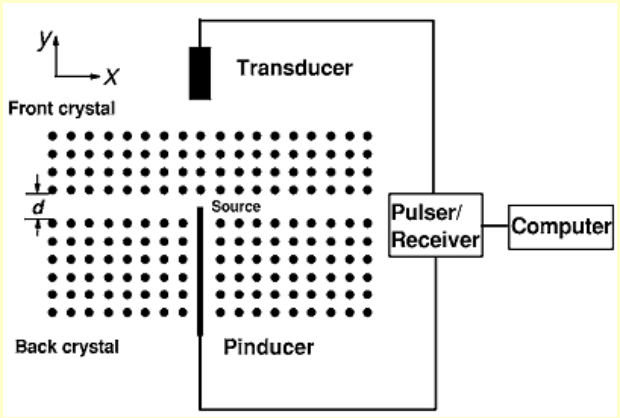
Silent outside in frequency regions of band gaps

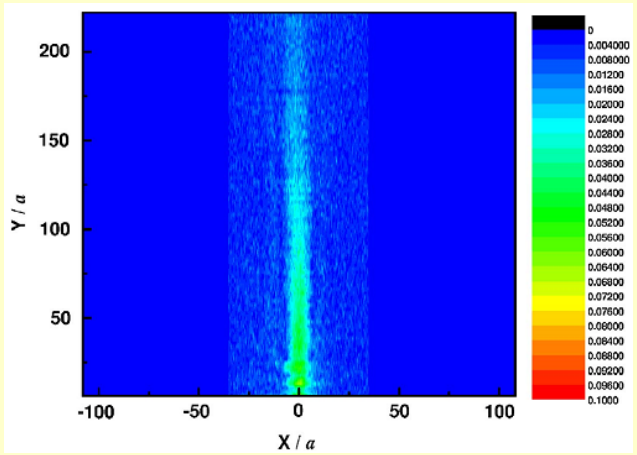
广阔的应用前景-2

定向辐射



Qiu, et al. APL, 2006 (Steel/Water)

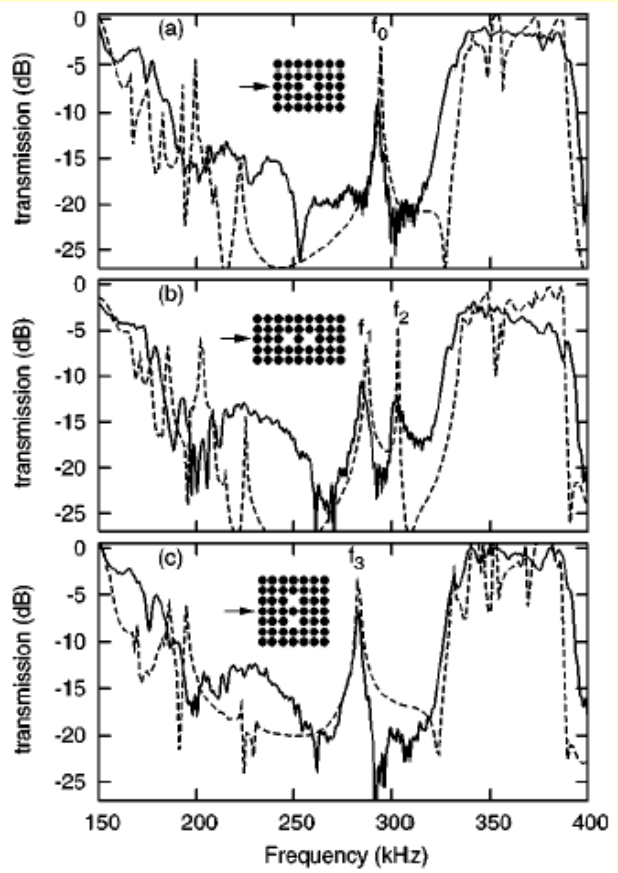


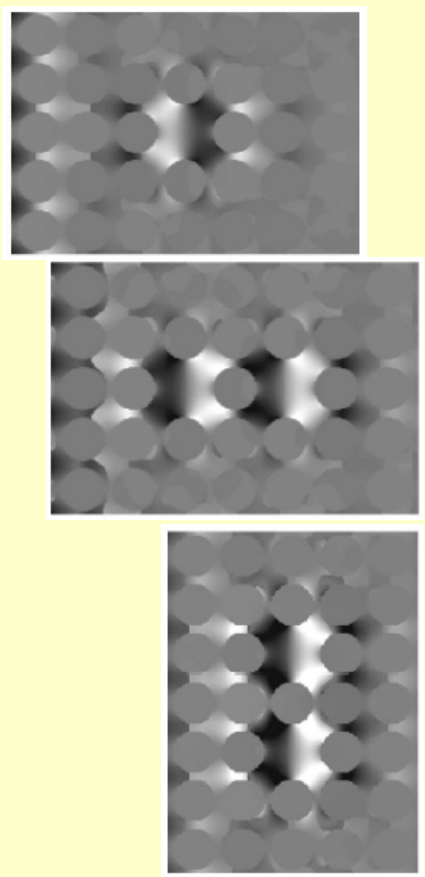


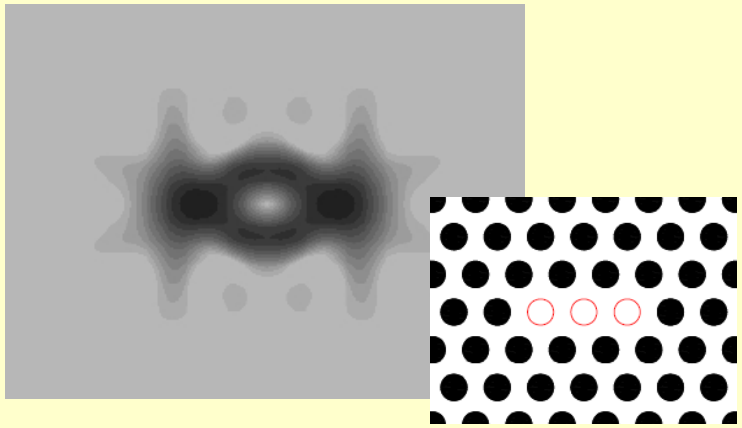
Ke, et al. APL
2006 (Steel/Water)

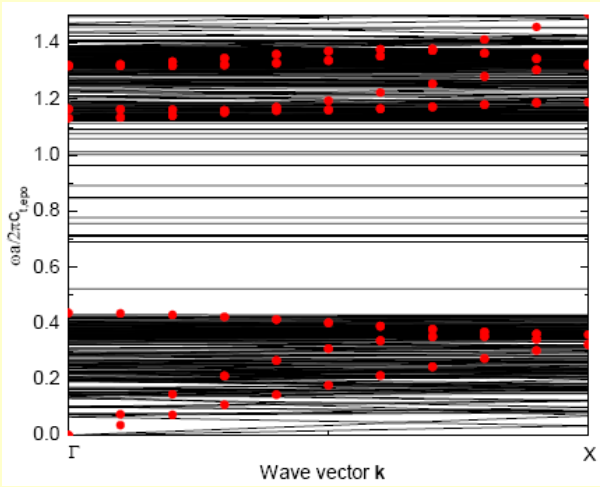
广阔的应用前景-3

点缺陷 ⇔ 波局域化 ⇔ 微谐振腔







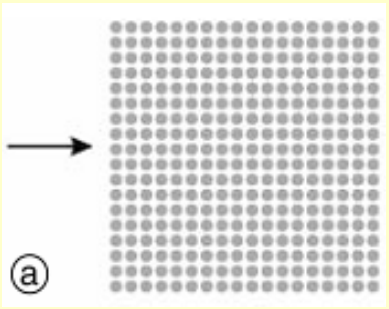


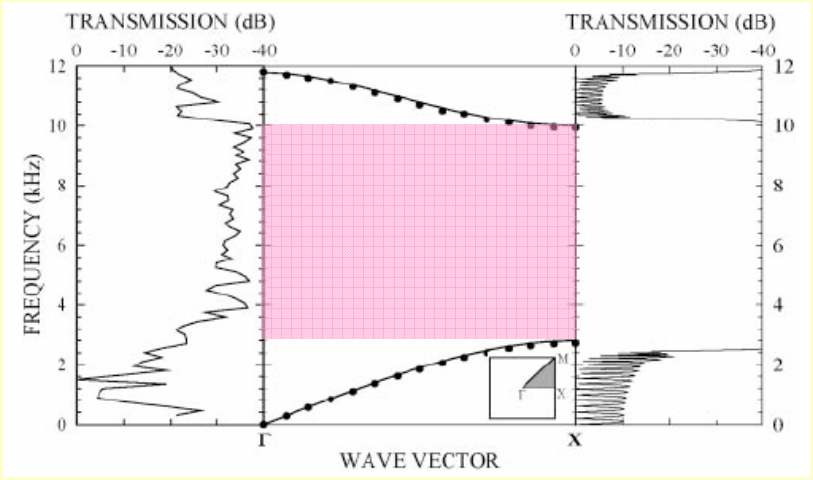
响应谱 (Steel/Water)
Khelif, et. al. PRB, 2003

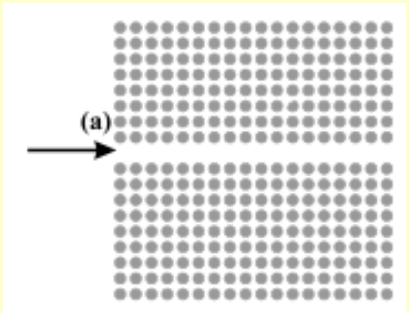
李建宝等, 人工晶体学报, 2010

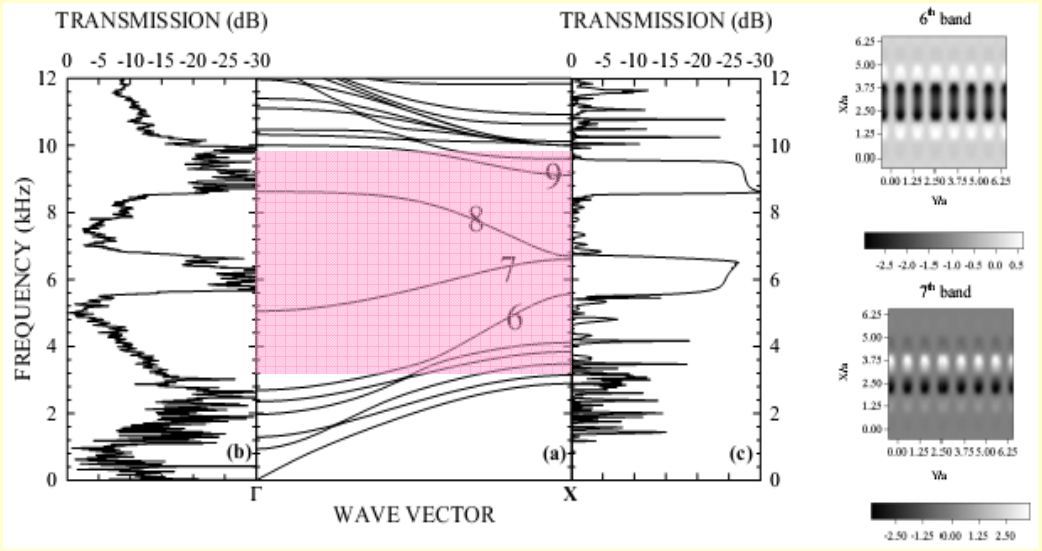
广阔的应用前景-4

线缺陷 ⇔ 波局域化 ⇔ 波导









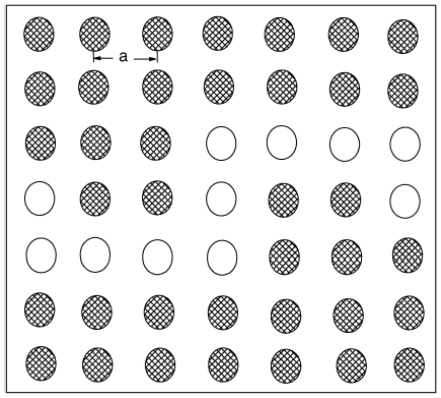
PVC/air

Vasseur, et al. Z. Kristallogr, 2005

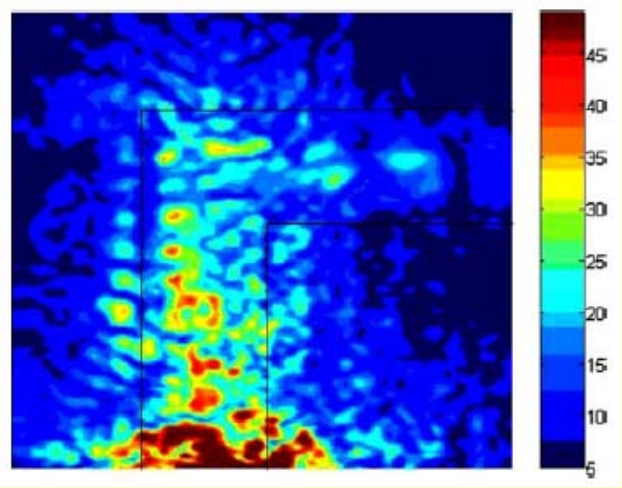
广阔的应用前景-5

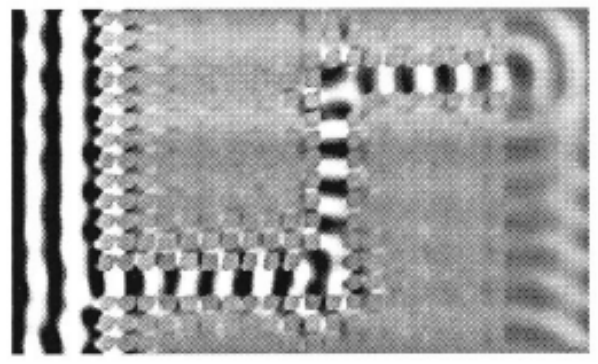
弯曲波导

Zhang, et. al. SSC, 2004 (Water/Hg)

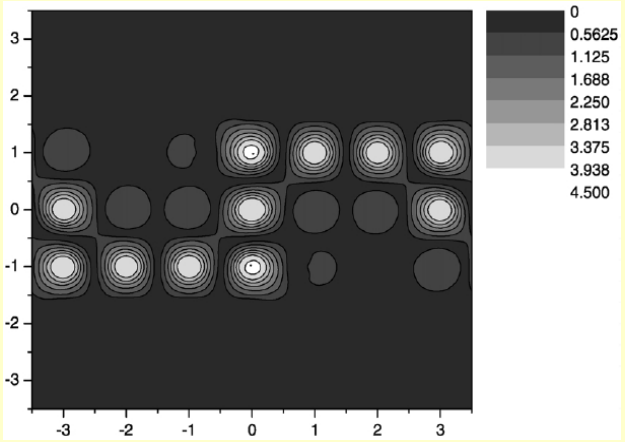


Torres, et.al. Ultrasonic 2004 (Hg/Al)





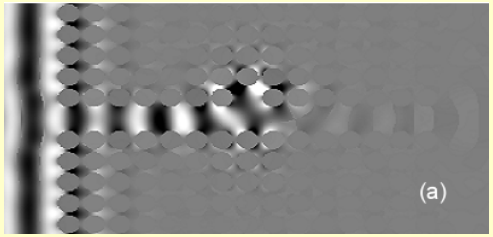
Khelif, et. al. APL 2004(Steel/Water)

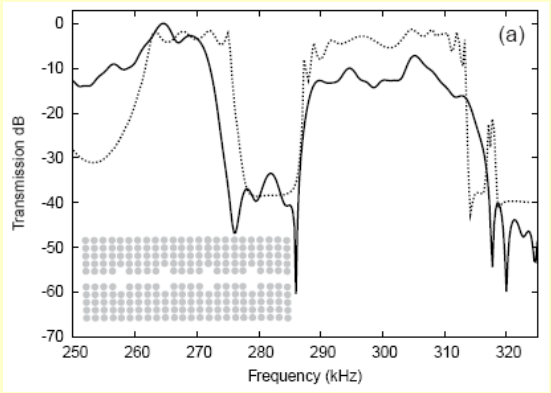


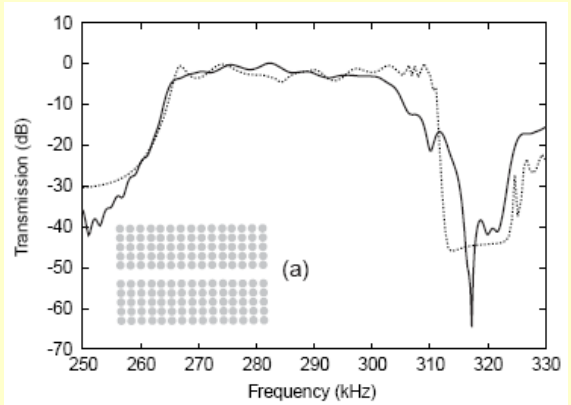
广阔的应用前景-6

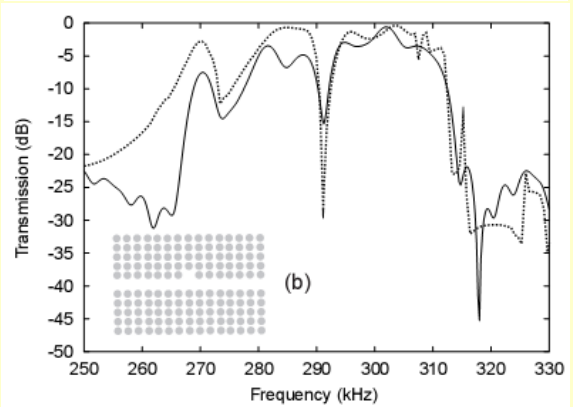
上/下载滤波器

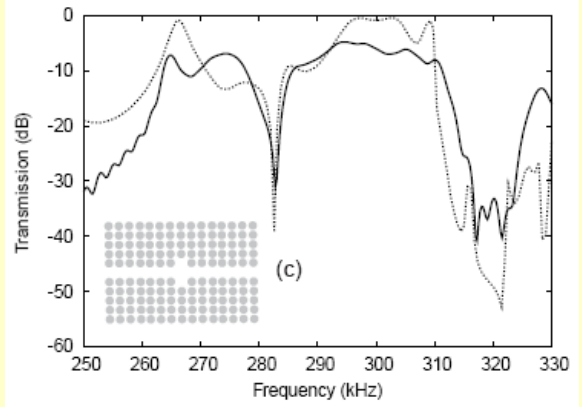
倍/分频器







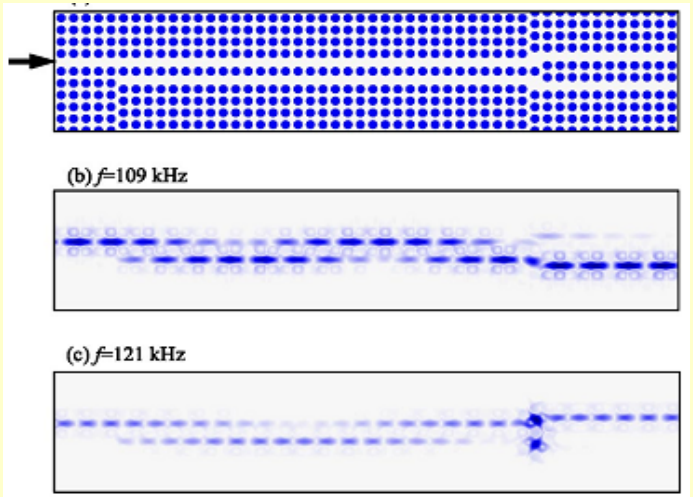




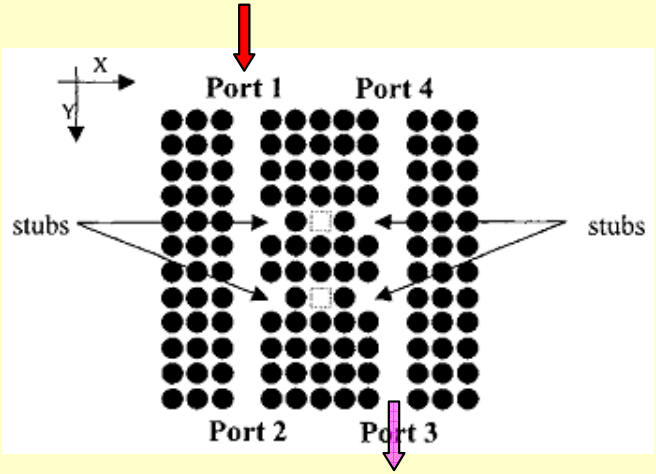
Benchabane, et al.
EPL, 2005 (Steel/Water)

广阔的应用前景-7

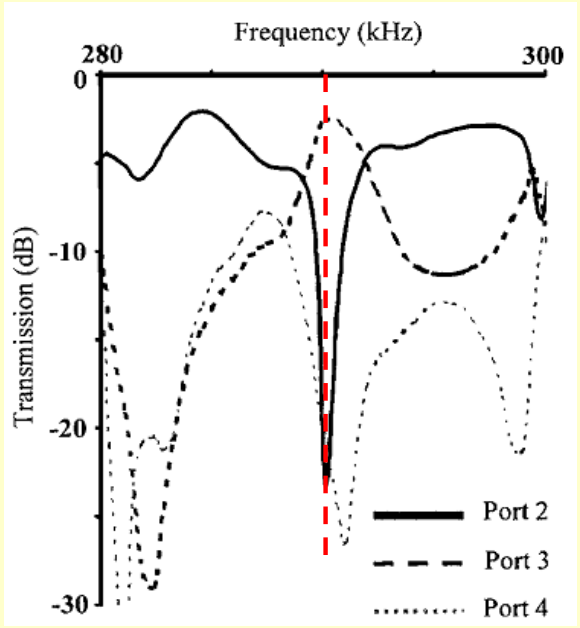
耦合器

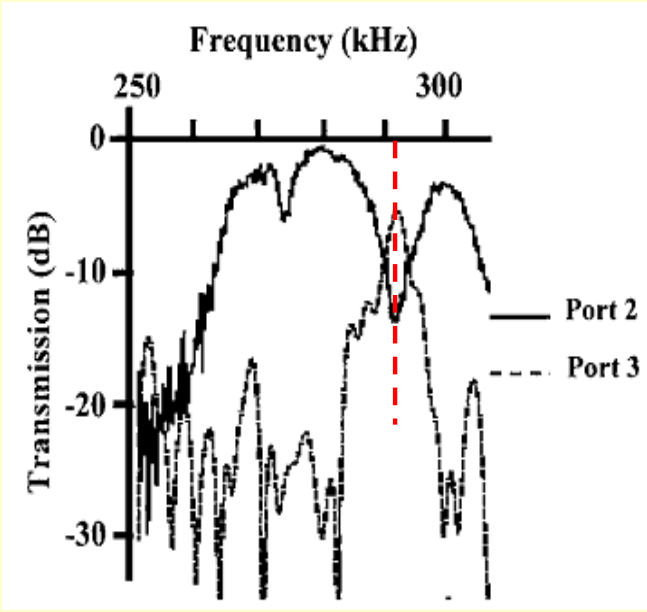


Sun, et al. PRB 2005(Steel/Epoxy)



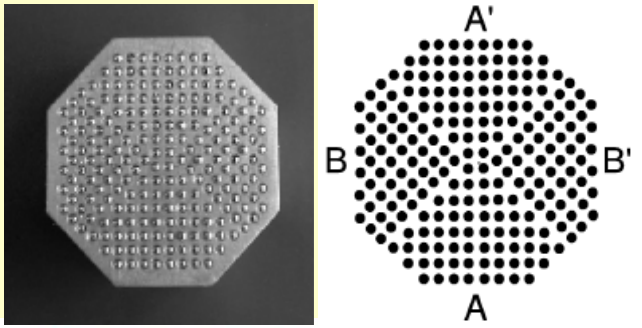
Pennec, et al. APL 2005(Steel/Water)

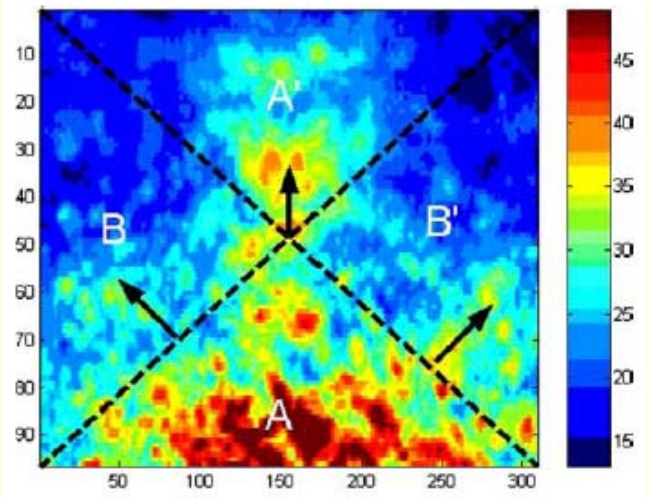




广阔的应用前景-8

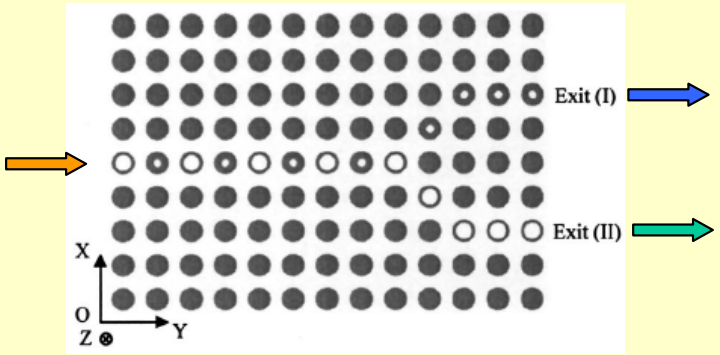
分离器

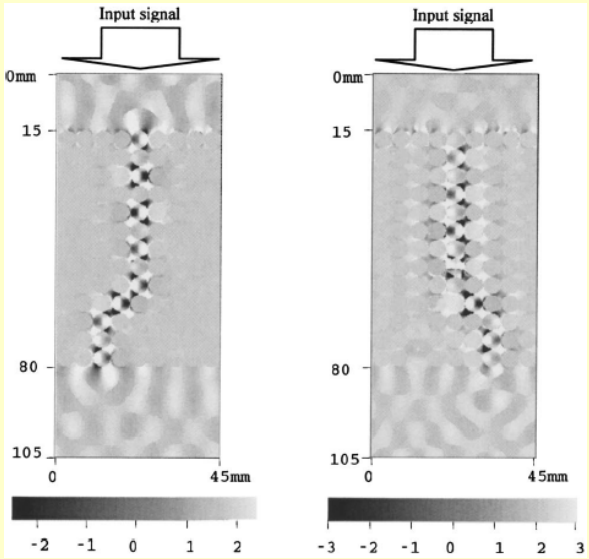




Torres, et.al. Ultrasonic, 2004 (Hg/Water)

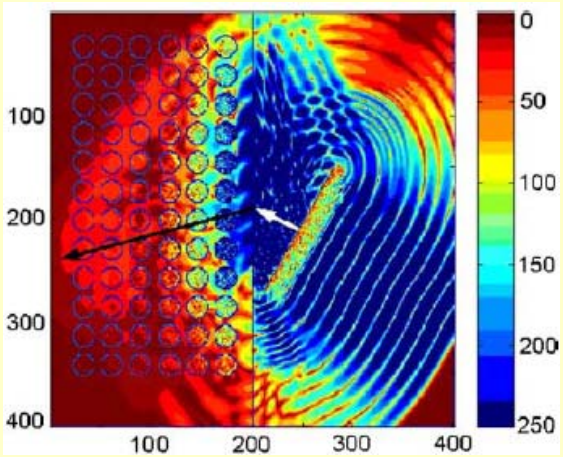
Pennec, et. al. PRE, 2004 (Steel/Water)



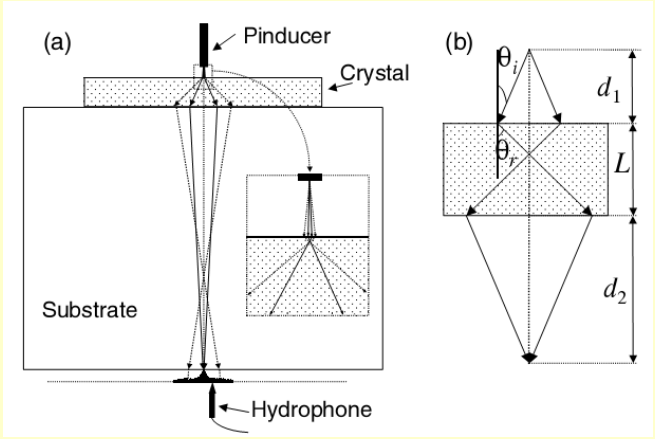


广阔的应用前景-9

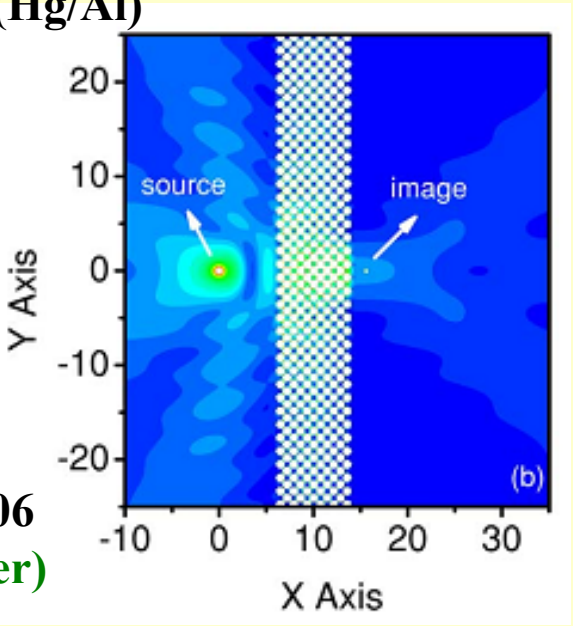
负折射 ⇔ 聚焦和成像 ⇔ 平板透镜



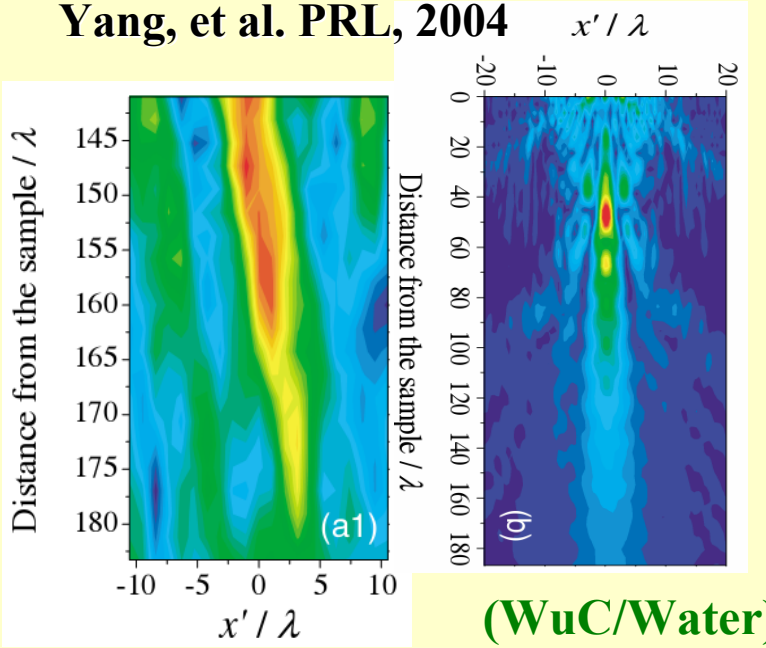
Torres, et.al.
Ultrasonic, 2004 (Hg/Al)



Yang, et al. PRL, 2004



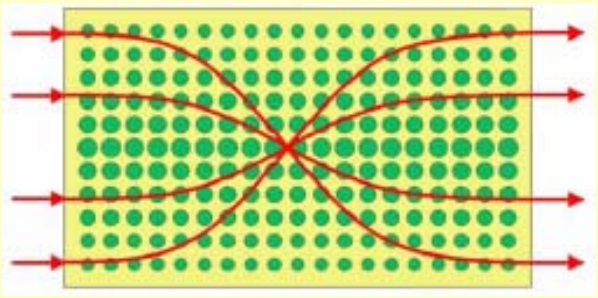
Li, et al. PRB, 2006
(Wu/Rubber/Water)

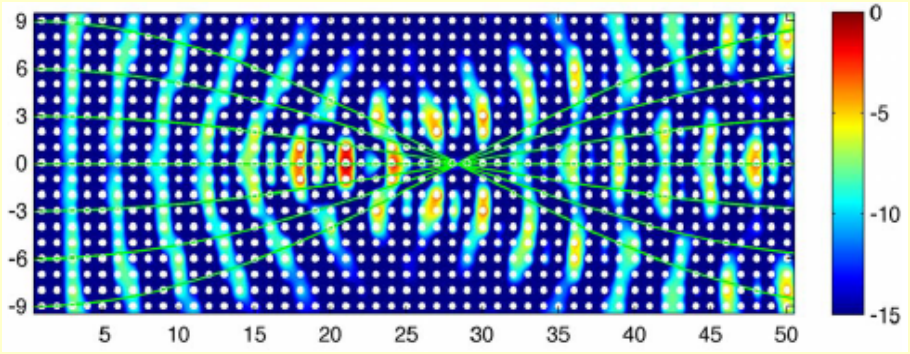


(WuC/Water)

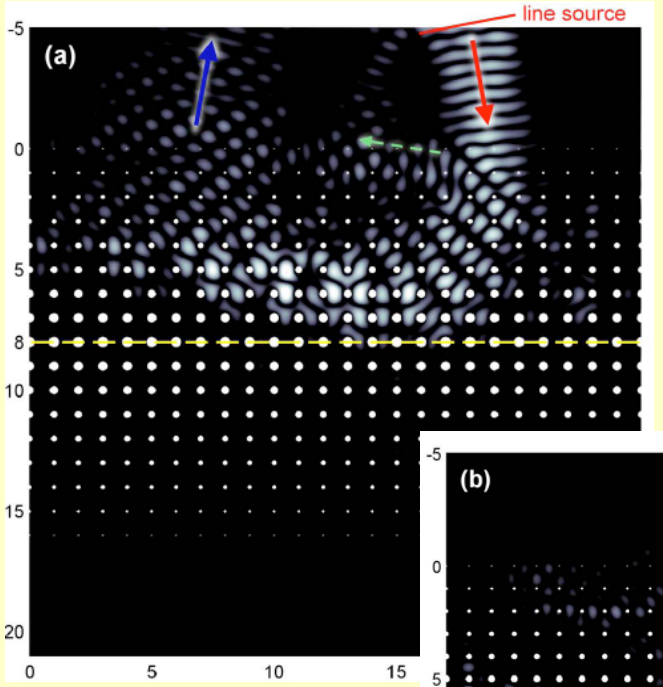
广阔的应用前景-10

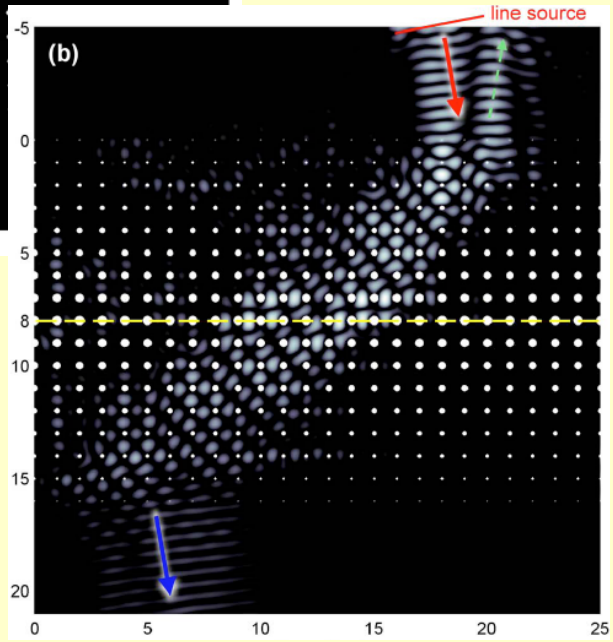
梯度声子晶体
控制传播路径





Lin, et al. PRB, 2009

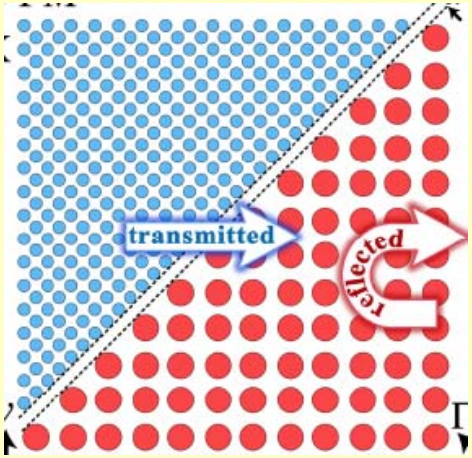


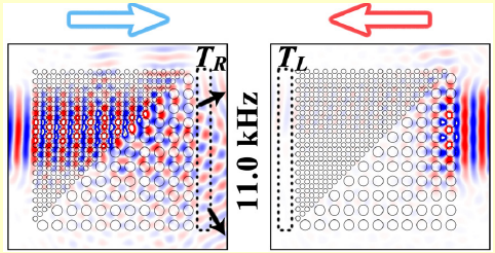


Lin, et al. JAP, 2009

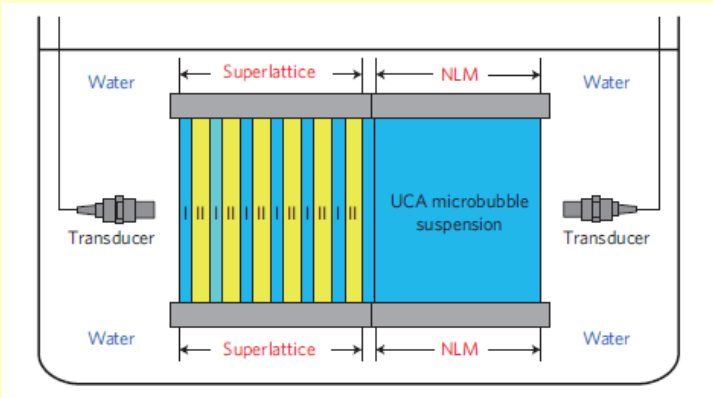
广阔的应用前景-11

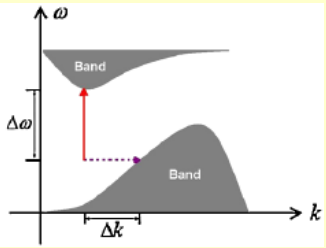
声整流器（二极管）



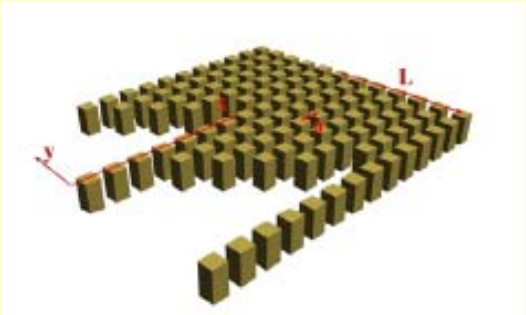


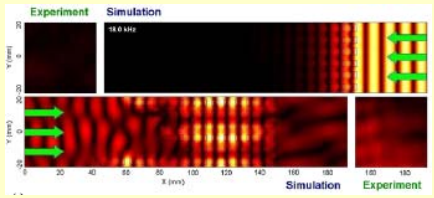
Junction diode
利用双声子晶体折射
Cicek, et al. APL, 2012



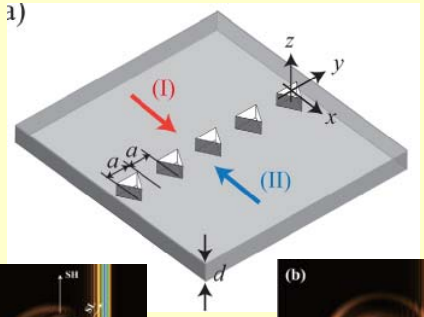


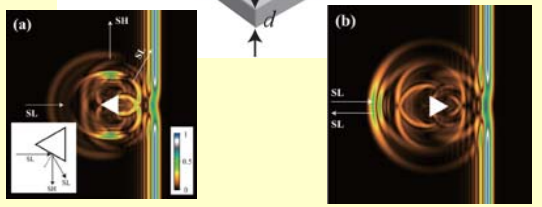
利用非线性材料
Liang, et al. Nat. Mat. 2010





Li, et al. PRL, 2011





Tanaka, et al. JAP, 2012

利用折射/反射

广阔的应用前景-12

(9) 其他

隧道效应、多谱勒效应、……

谐振器、传感器、集能器、声学隐身、……

广阔的应用前景-13

鱼群探测

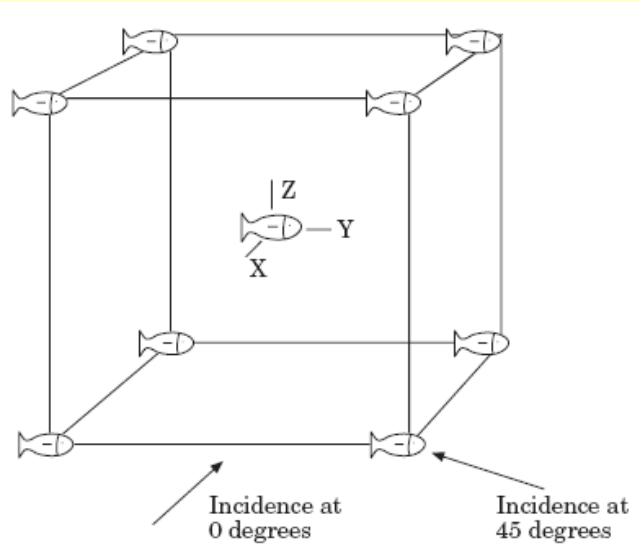
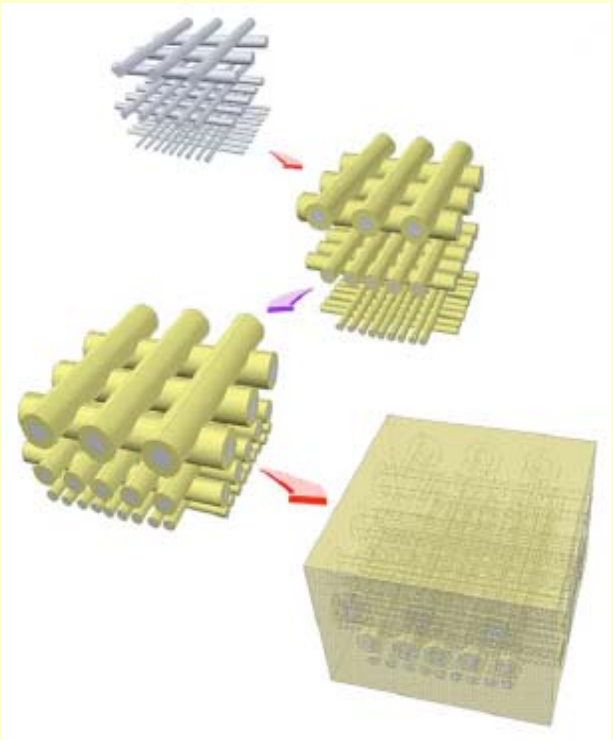


Figure 1. A body centred fish school unit.

Alvarez, ICES_JMS, 1999

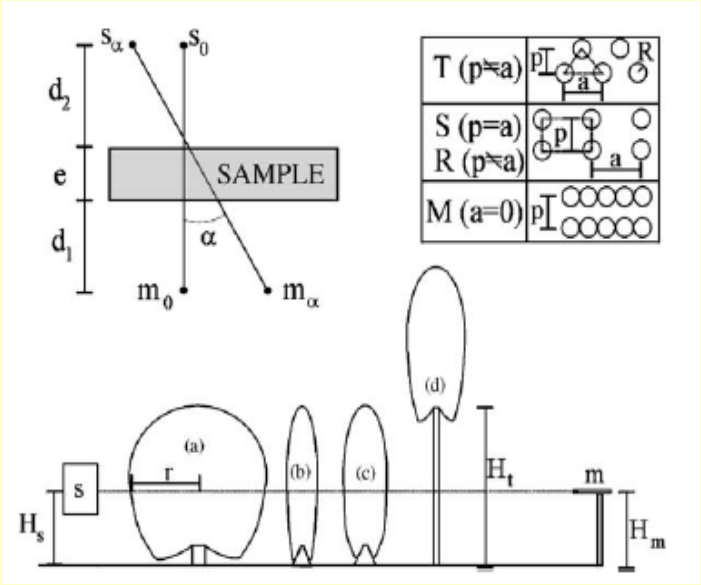
拓 展

水声吸收



Jiang, et al. APL, 2009

树木隔音



Martınez-Sala, et al. JSV, 2006

带隙调控-1

带隙特征(位置、宽度、方向等)的决定参数：

晶格排布、晶格尺寸
散射体形状、填充比
组合材料（固/液/气）
材料参数比（密度/模量/声阻抗）
单元共振特性……

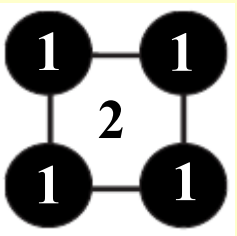
超强的可设计性！ — 优化

带隙工程： 调节材料和结构参数 ⇒ 调制带隙

⇒ 操控波的传播 ⇒ 设计声学器件

带隙调控-2

材料参数对带隙的调制（2维固/固）：



$$-\bar{\omega}^2\bar{\rho}(\mathbf{r})u_\alpha(\mathbf{r})=[\kappa_2\bar{\lambda}(\mathbf{r})u_{\beta,\beta}(\mathbf{r})]_{,\alpha}+\{\bar{\mu}(\mathbf{r})[u_{\alpha,\beta}(\mathbf{r})+u_{\beta,\alpha}(\mathbf{r})]\}_{,\beta},\quad \alpha,\beta=x,y,$$

平面混合模态

$$-\bar{\omega}^2\bar{\rho}(\mathbf{r})u_z(\mathbf{r})=\nabla[\bar{\mu}(\mathbf{r})\nabla u_z(\mathbf{r})]$$

反平面横波模态

$$\bar{\rho}(\mathbf{r})=\begin{cases}1, & \mathbf{r}\in\Omega_2\\ \rho_1/\rho_2 & \mathbf{r}\in\Omega_1\end{cases}$$

$$\bar{\mu}(\mathbf{r})=\begin{cases}1, & \mathbf{r}\in\Omega_2\\ \mu_1/\mu_2, & \mathbf{r}\in\Omega_1\end{cases}$$

$$\bar{\lambda}(\mathbf{r})=\begin{cases}1, & \mathbf{r}\in\Omega_2\\ \lambda_1/\lambda_2, & \mathbf{r}\in\Omega_1\end{cases}$$

$$\lambda_1/\lambda_2=(\mu_1/\mu_2)(\kappa_1/\kappa_2)\qquad \kappa_1=2\nu_1/(1-2\nu_1)$$

$$c_{t1}/c_{t2}=\sqrt{(\mu_1/\mu_2)/(\rho_1/\rho_2)}$$

$$z_{t1}/z_{t2}=\sqrt{(\mu_1/\mu_2)(\rho_1/\rho_2)}$$

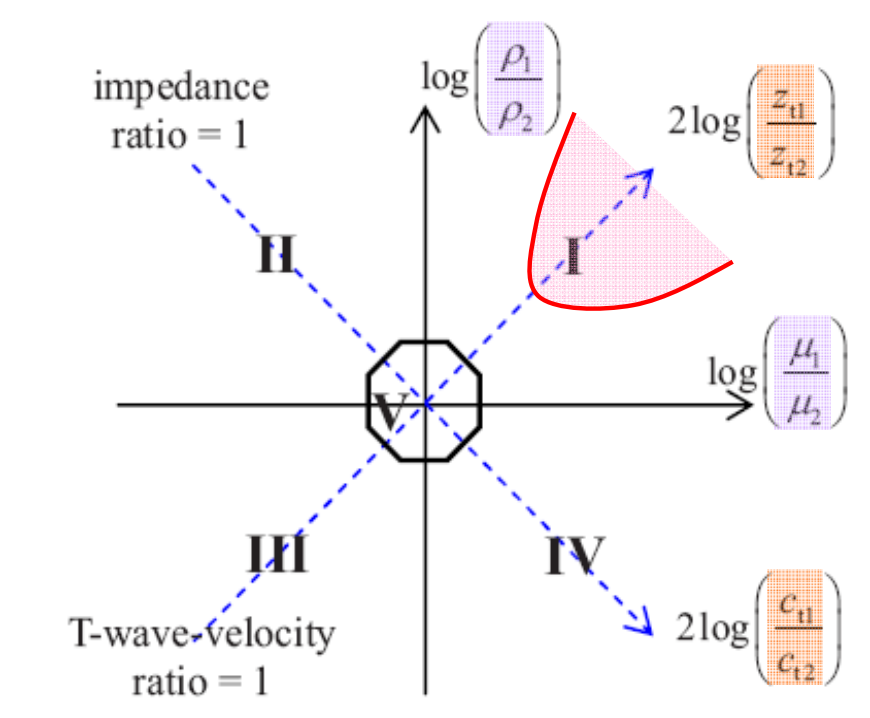
密度比 ρ_1/ρ_2，或速度比 c_{t1}/c_{t2}

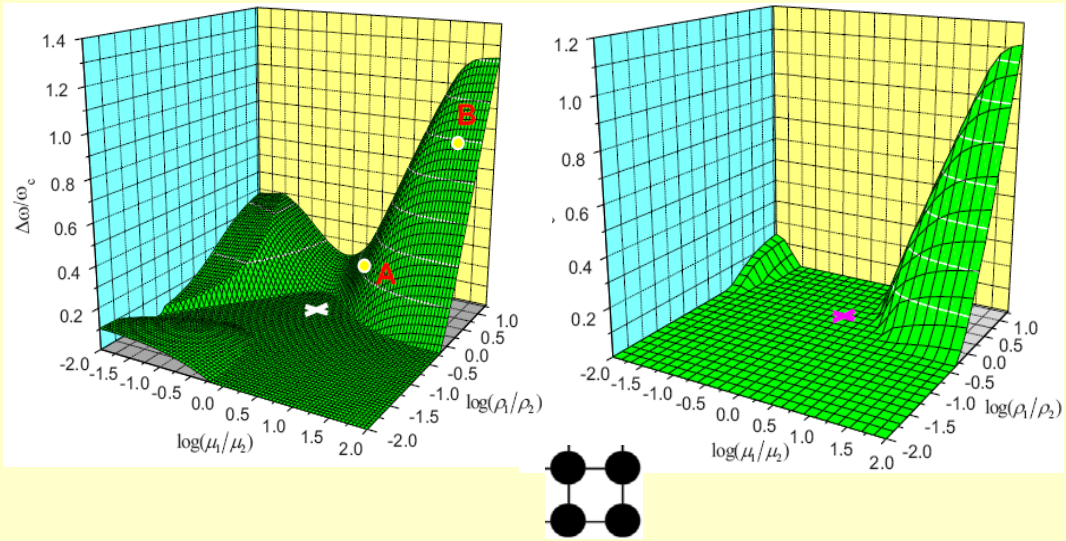
模量比 μ_1/μ_2，或阻抗比 z_{t1}/z_{t2}

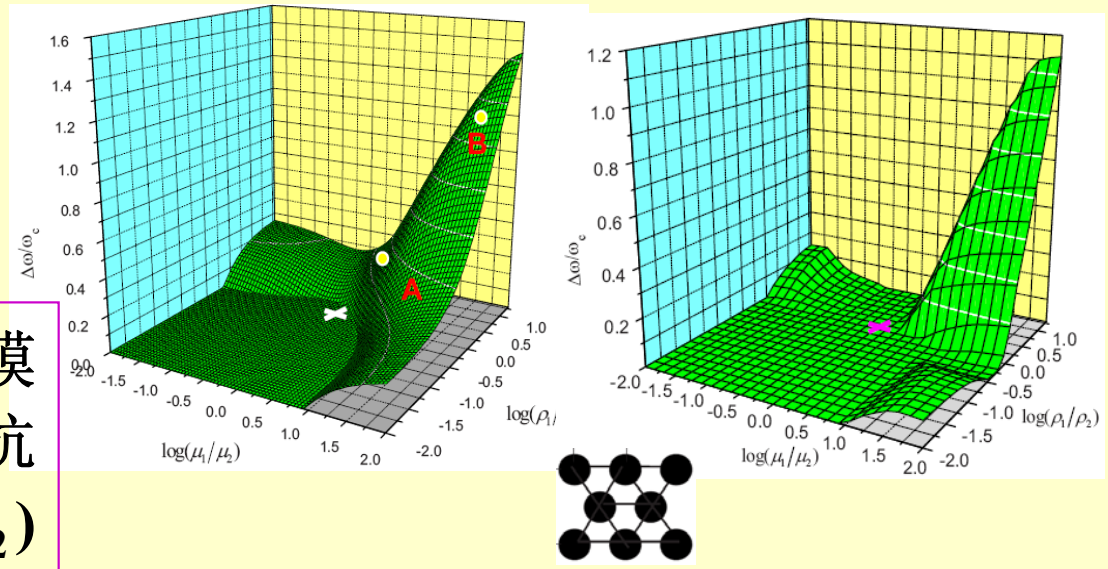
泊松比 ν_1 & ν_2。

带隙调控-3

材料参数平面:





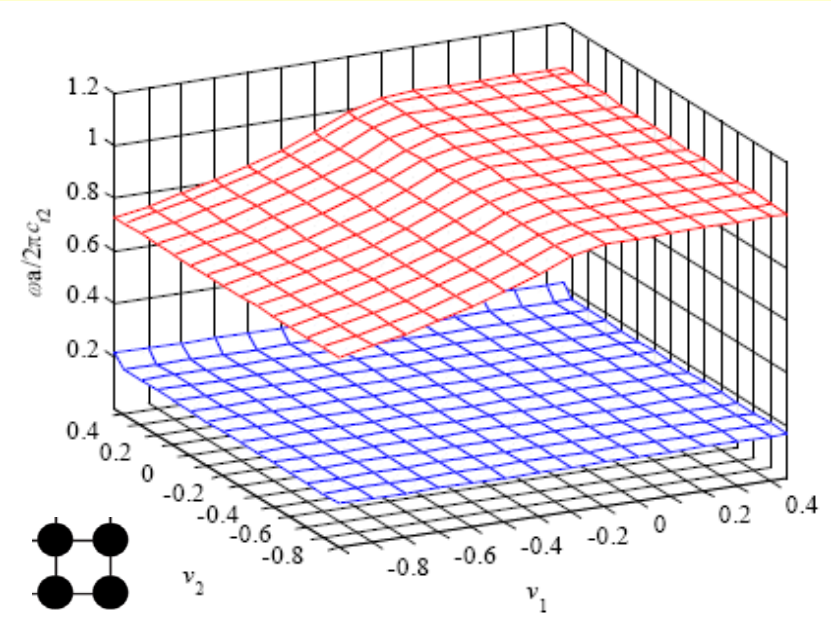


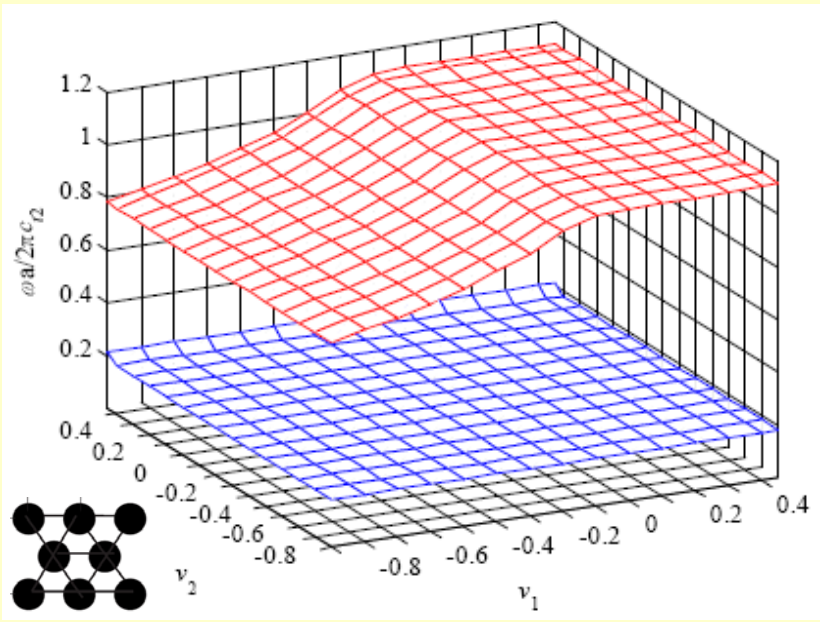
带隙主要出现在密度比(ρ_1/ρ_2)和模量比(μ_1/μ_2)都很大的情况，或阻抗比(z_{t1}/z_{t2})很大而速度比(c_{t1}/c_{t2})很小的情况，泊松比(正)影响不大

Zhou, Wang, Zhang, JAP, 2009

带隙调控-4

Poisson比的影响:

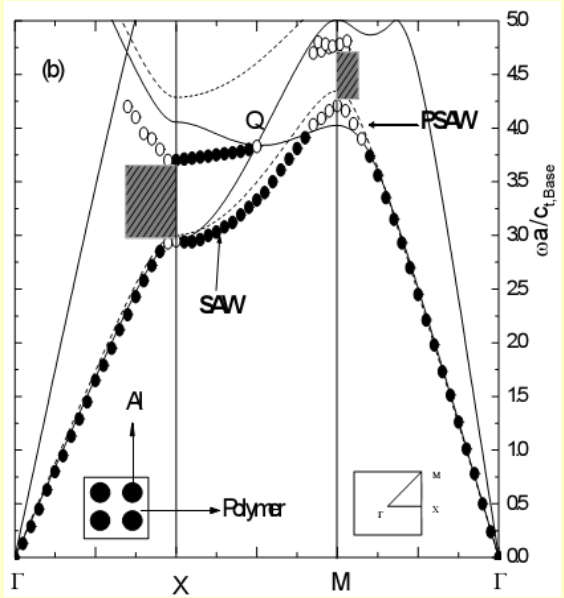




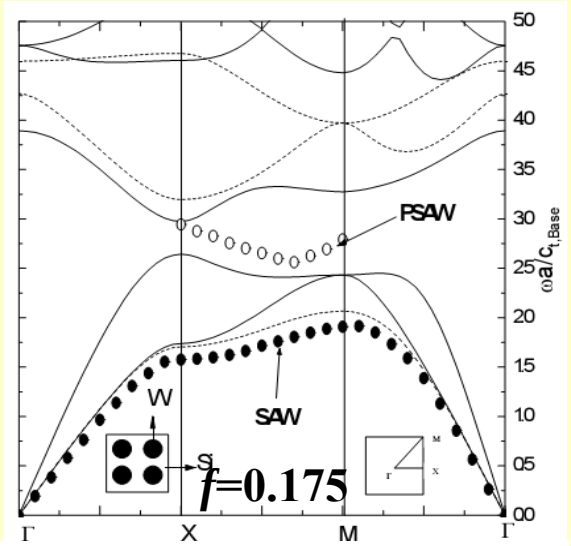
负的Piosson比对带隙宽度影响较大，且使带隙宽度减小。

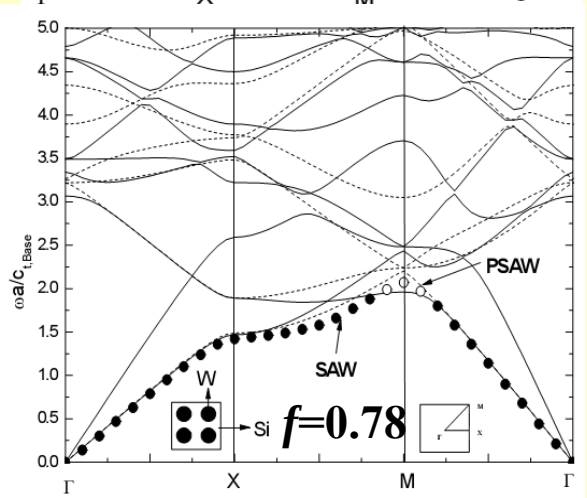
Ma, Wang, Su, Phys. B, 2012

带隙调控-5 表面波

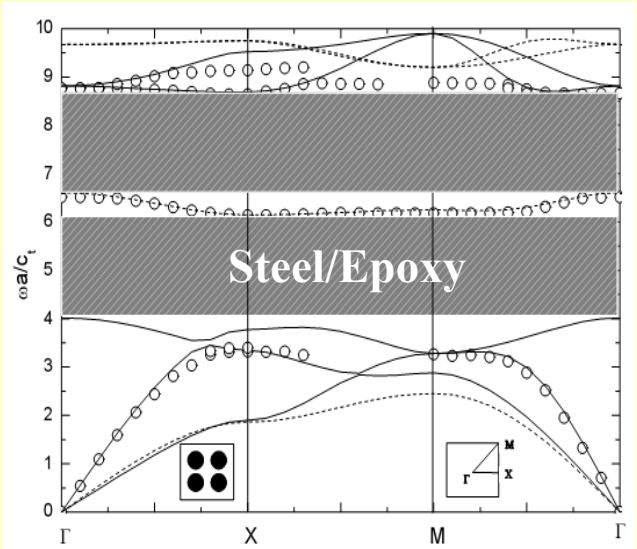


2.7/2.5; f=0.6

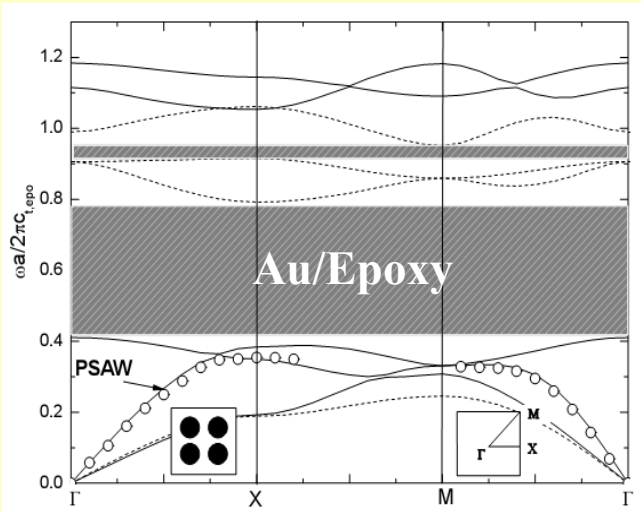




4.7/4.3



15.25/18.6; f=0.4



21.9/17.7; f=0.4

声阻抗比的影响：

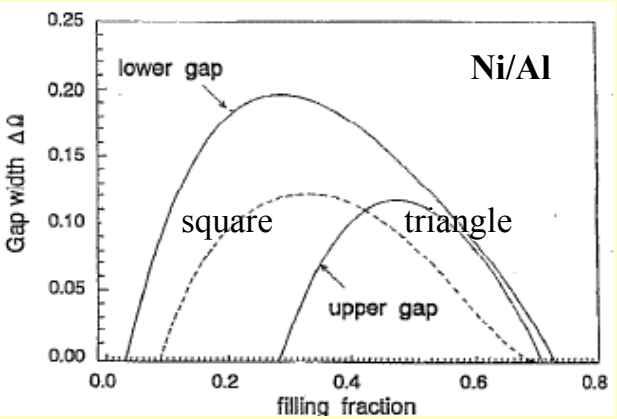
$$Z_s^L / Z_m^L \Big/ Z_s^T / Z_m^T$$

越大越不易出现表面波

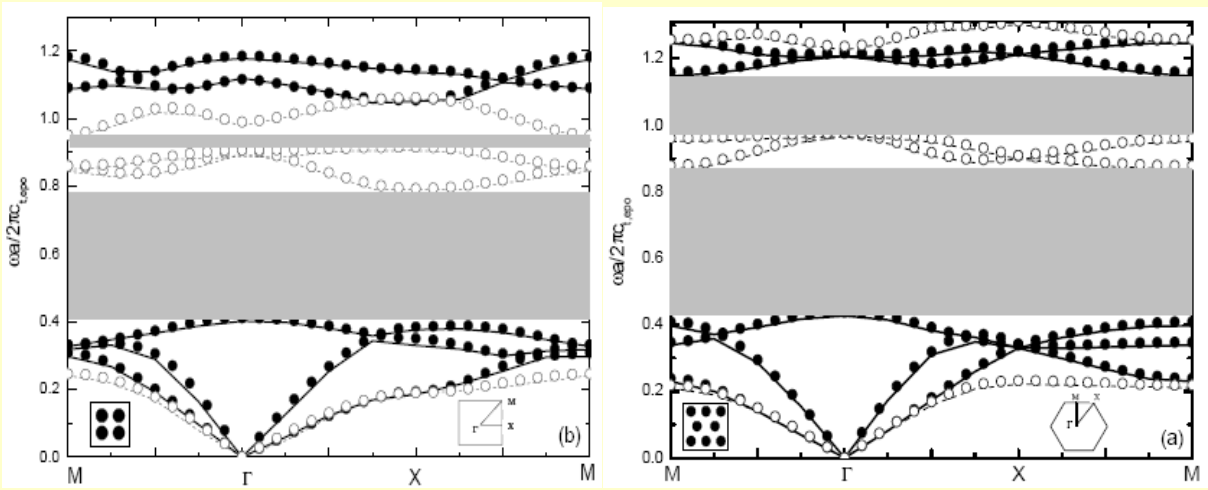
Yan, Wang, PRB, 2008

带隙调控-6

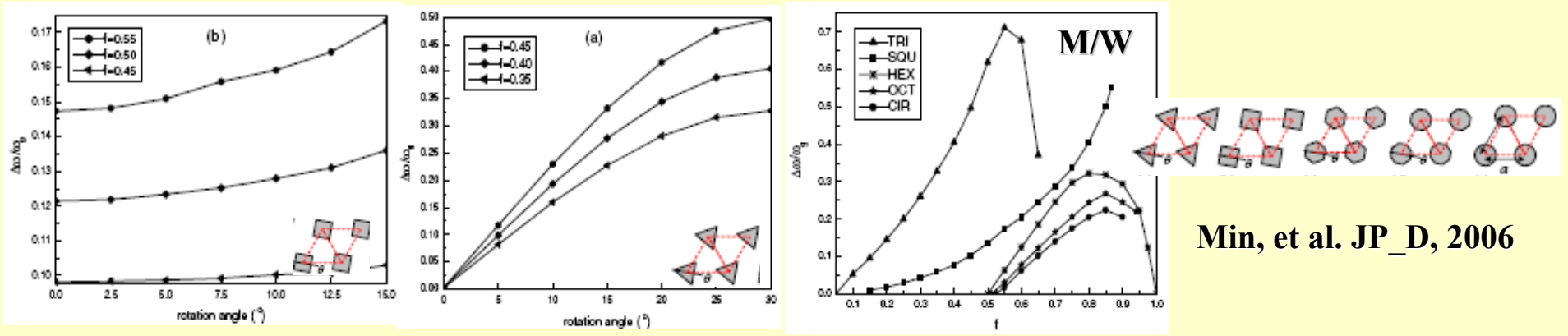
结构参数对带隙的调制：填充比、晶格排布、散射体形状



Kushwaha, et al. APL, 1994

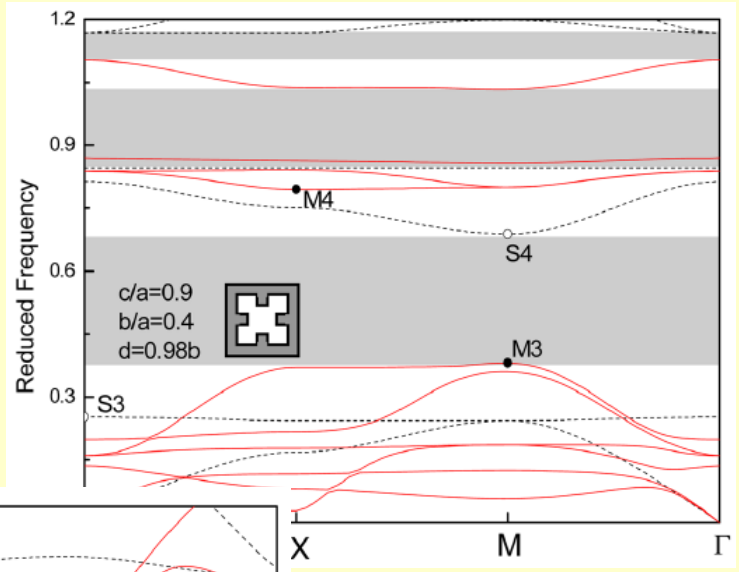


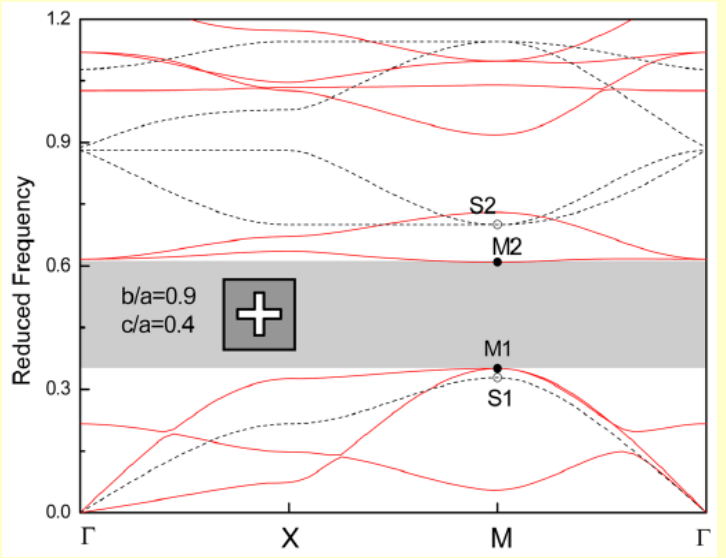
Yan, Wang, et al. CMES, 2008

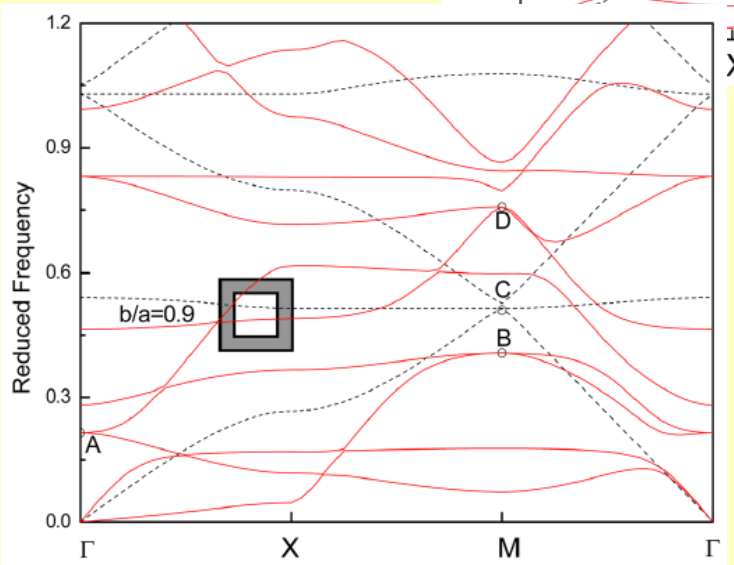


Min, et al. JP_D, 2006

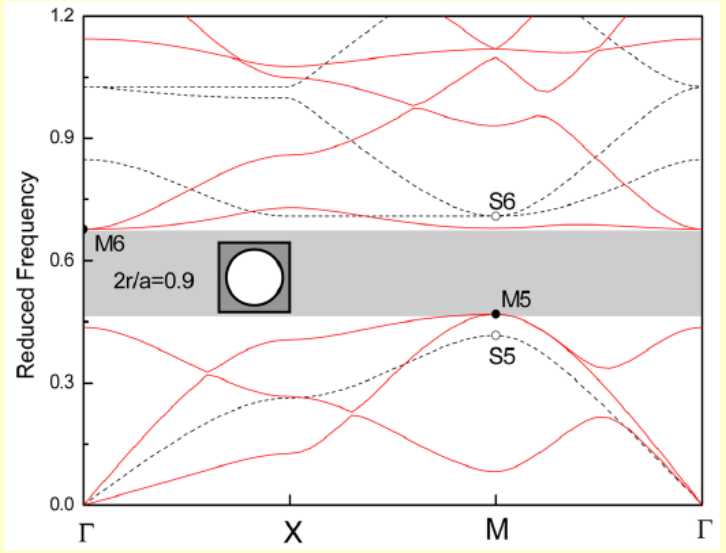
散射体（孔）形状对带隙的调控





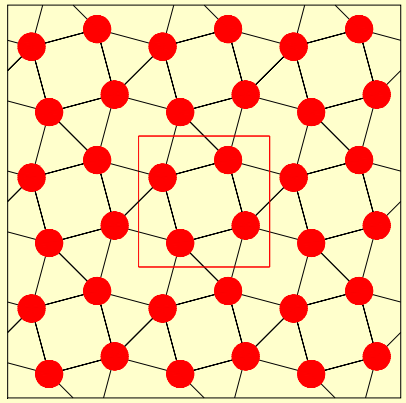


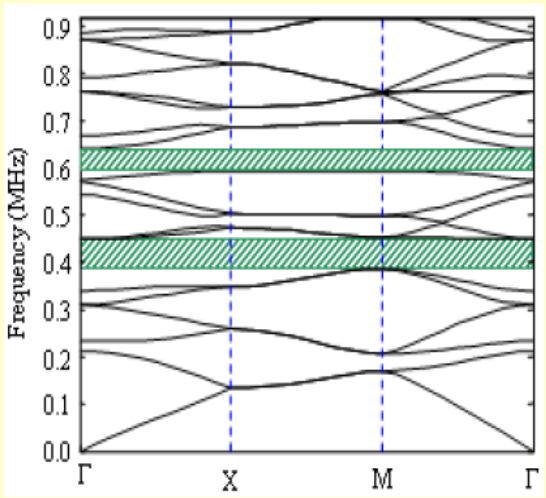
Wang, et al. JAP, 2012

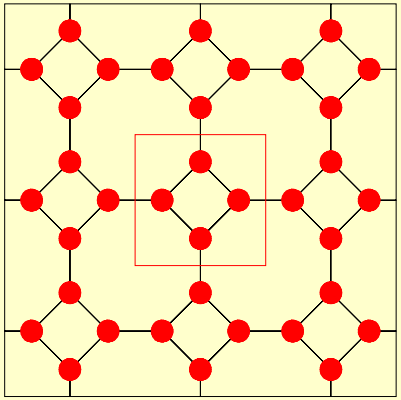


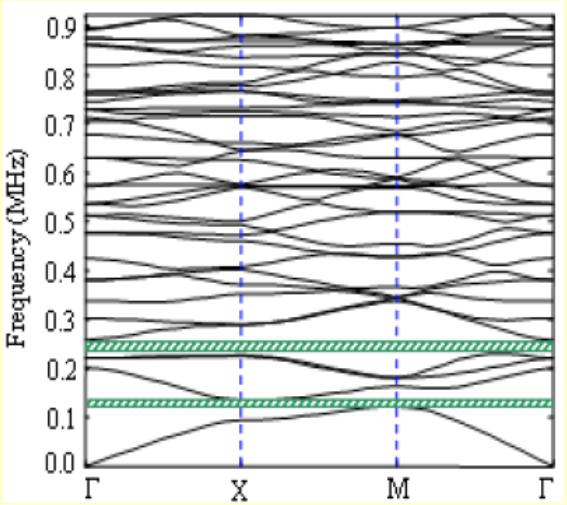
带隙调控-8

阿基米德格子



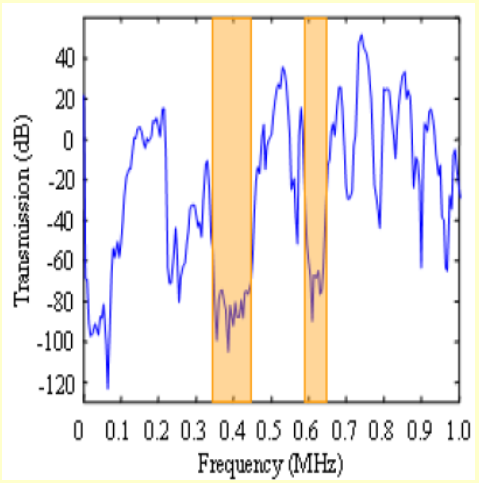


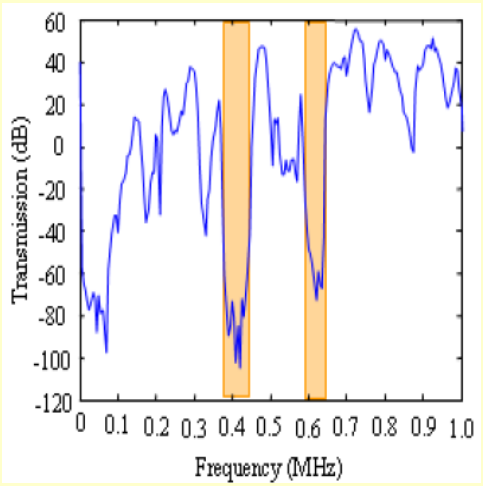


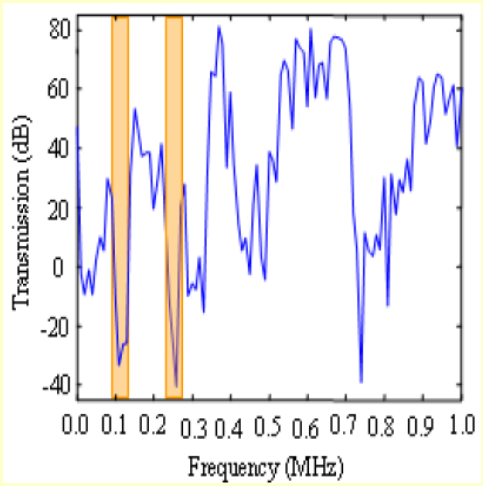


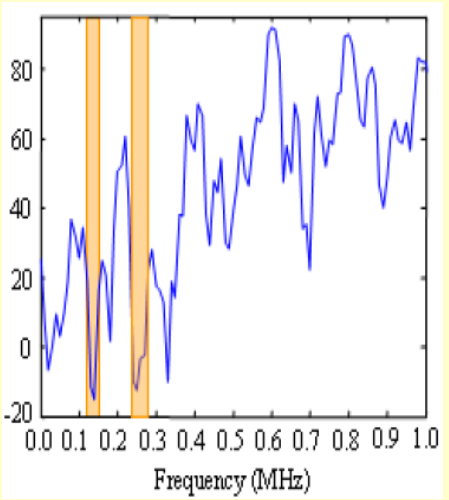




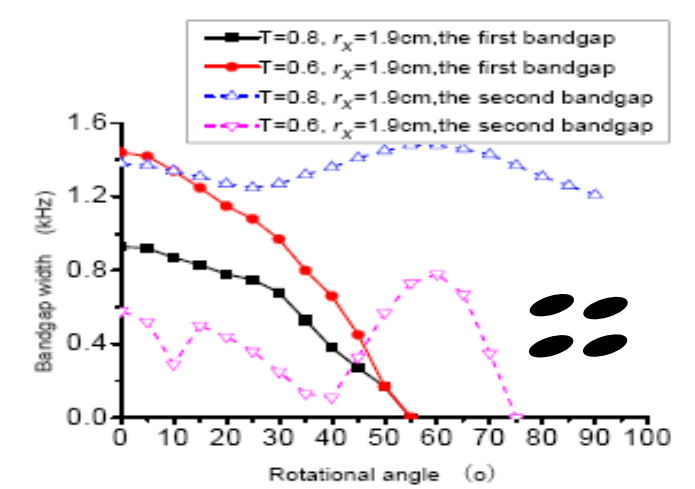


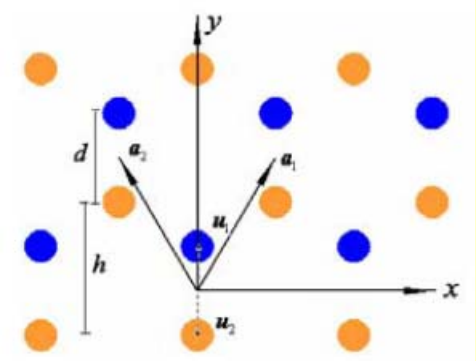


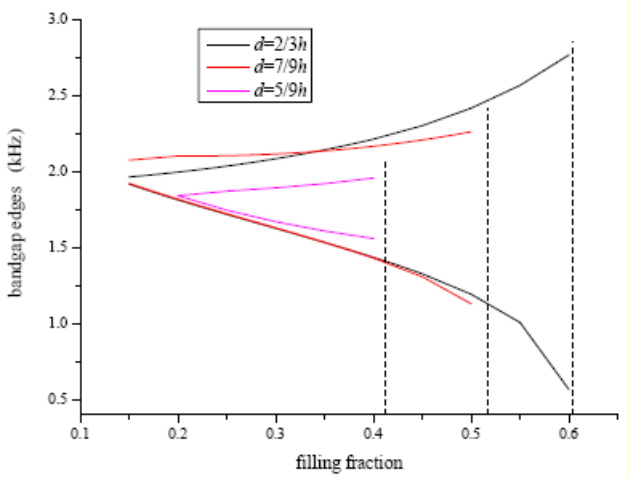




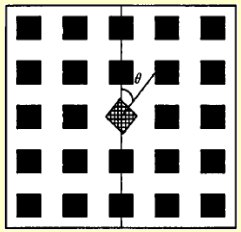
对称性对带隙和缺陷态的调制

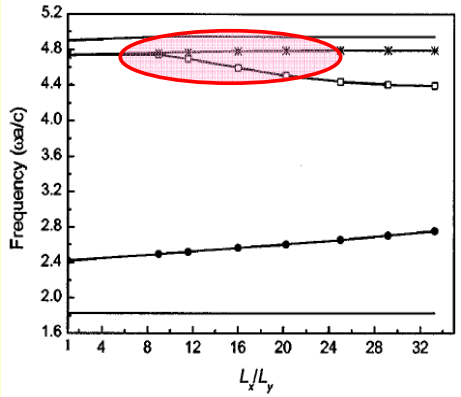




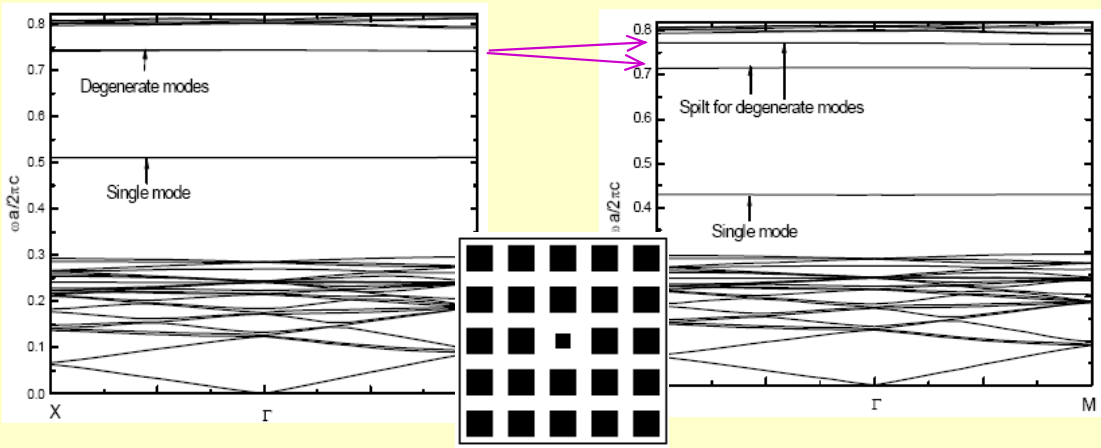


简并的缺陷模态分离





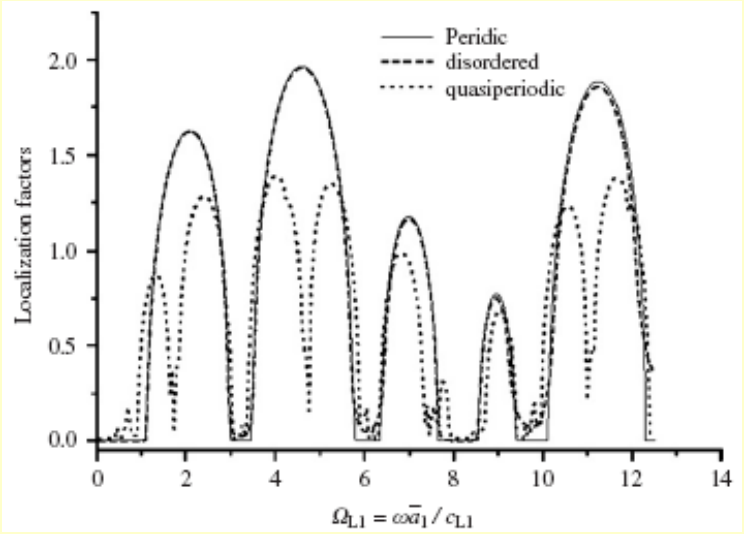
Wu, et al. PRE, 2004



闫志忠, 博士论文, 2008

准周期调制带隙

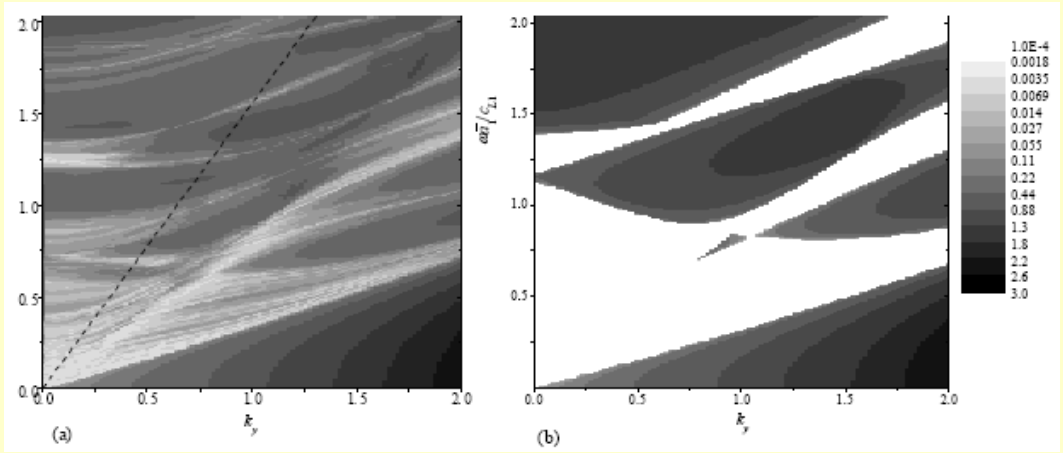
获得更多的带结构

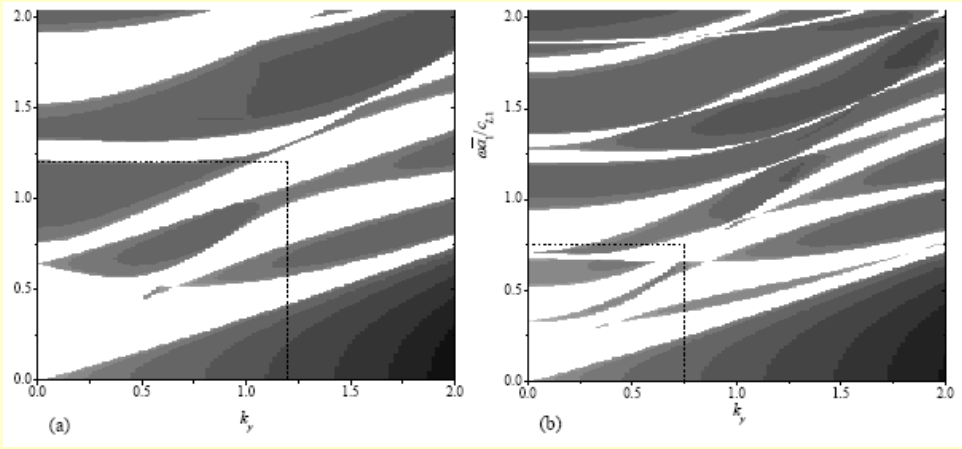


1-D, Pb/Epoxy

Chen, Wang, et al. SSC, 2007

准周期　　周期

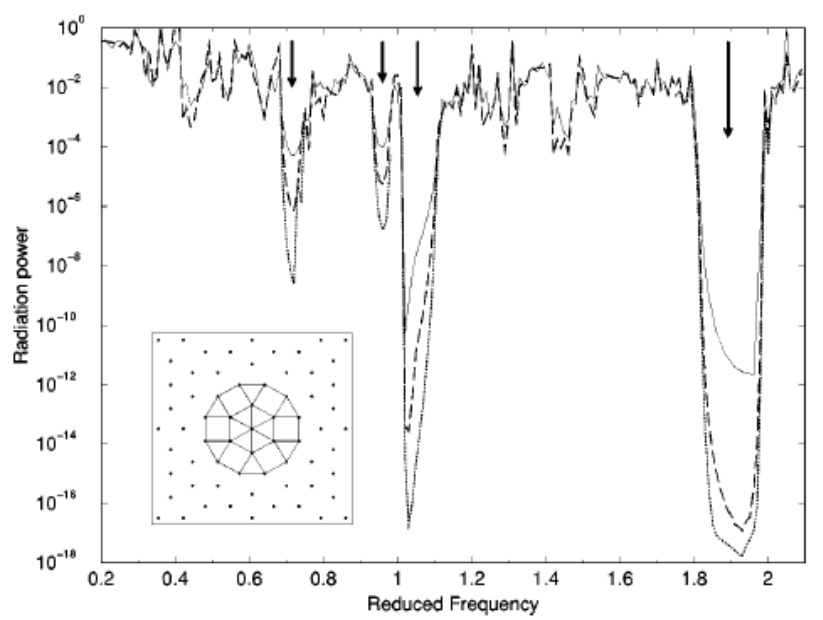


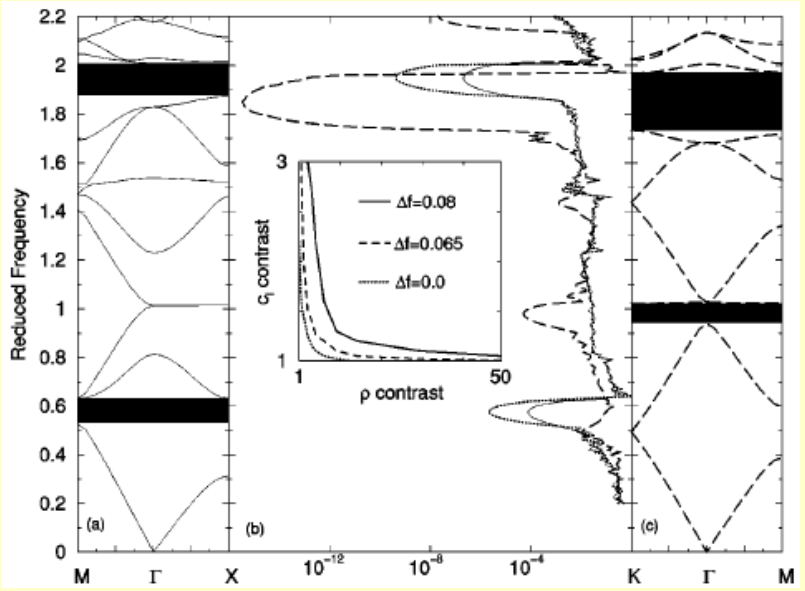


准周期+平移对称　　准周期+镜像对称+平移对称

带隙调控-11

准周期 (二维)





square **triangular**

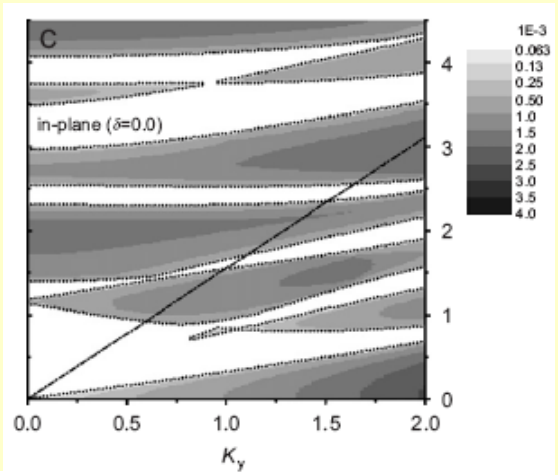
Lai, et al. JAP, 2002

钢/气，12重准晶

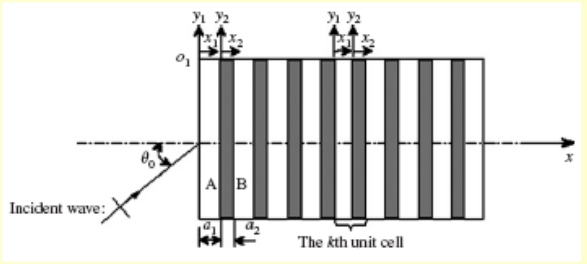
带隙调控-12

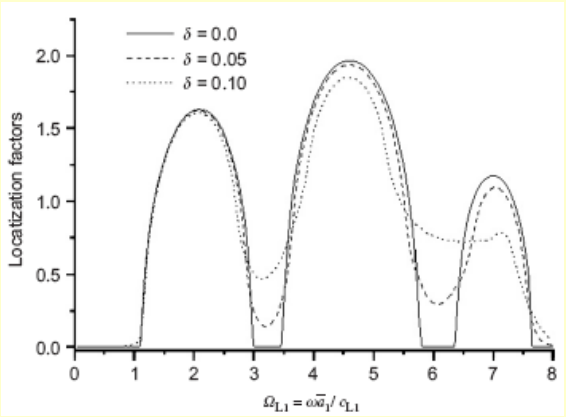
一定程度的随机失谐调制带隙

完全周期

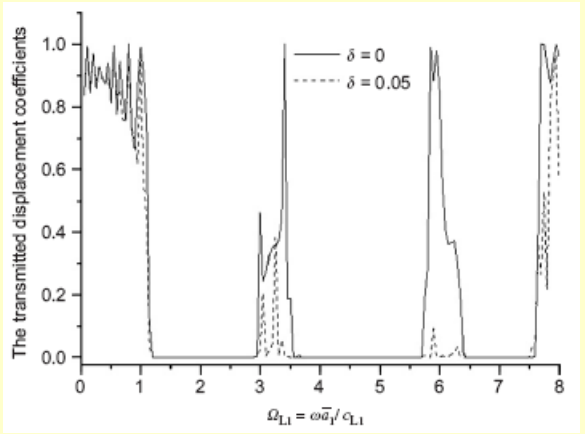


失谐度δ=.05





局部化因子



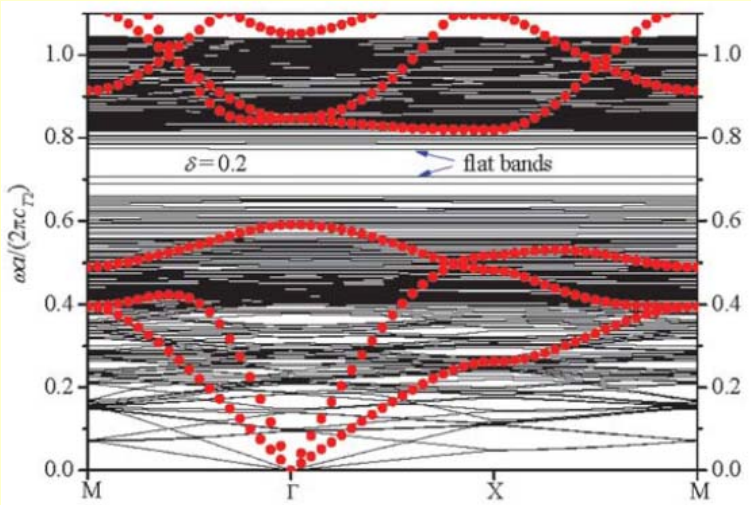
透射系数

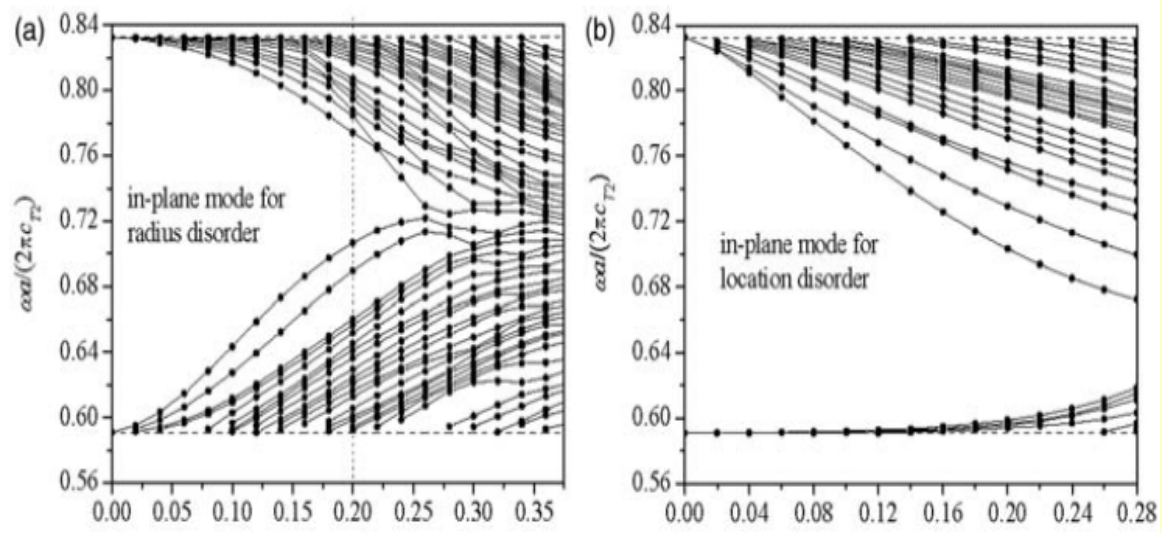
Chen, Wang, Physica B, 2007

(Pb/Epoxy)

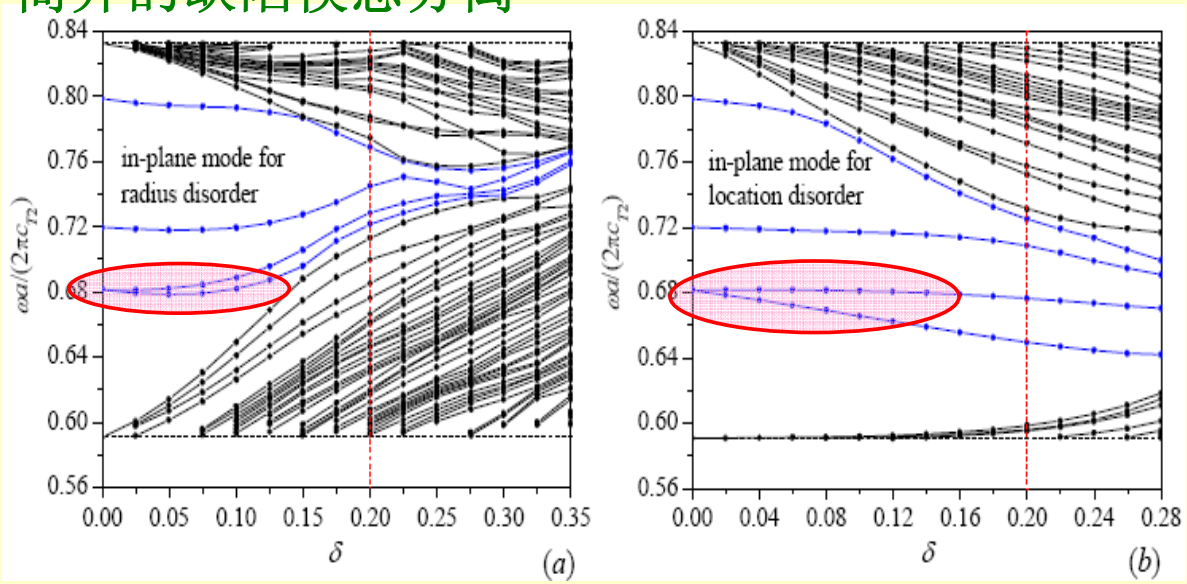
带隙调控-13

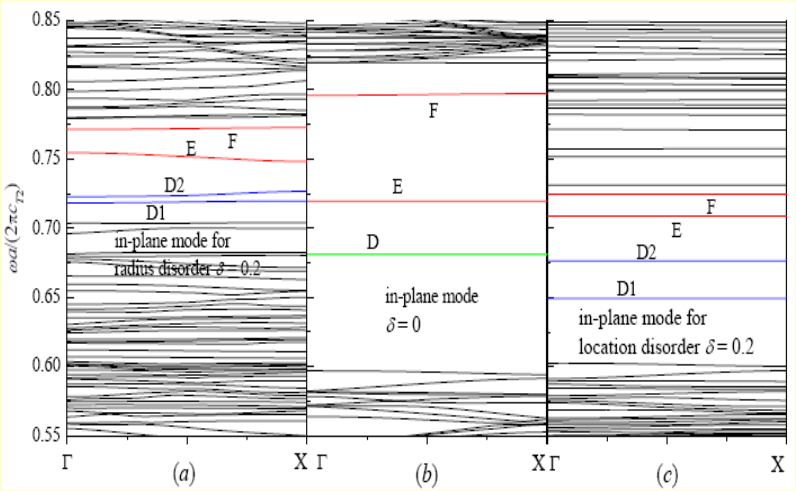
失谐对带隙和缺陷态的调制





简并的缺陷模态分离

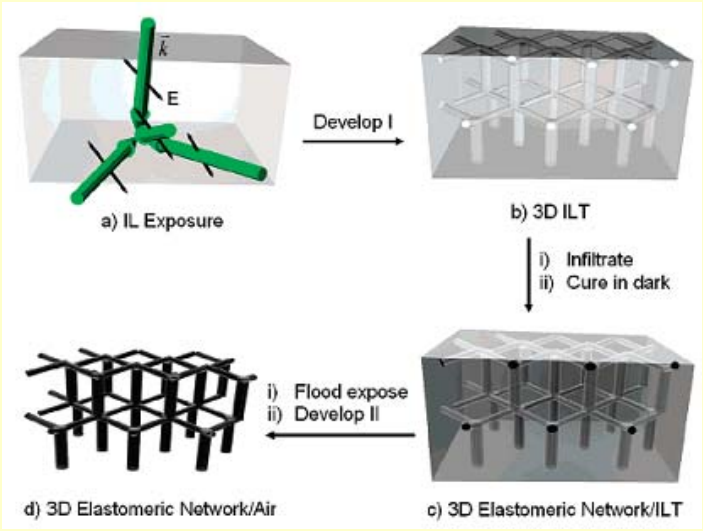




Chen, Wang, et al. WRCM, 2010

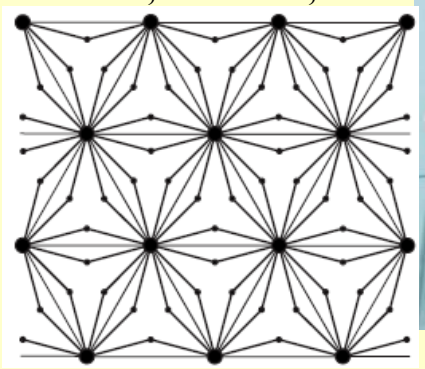
(Pb/Epoxy)

形形色色的声子晶体



Jang, etal. Nano L, 2006

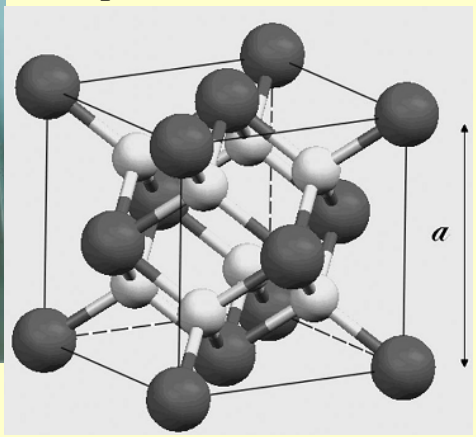
Yilmaz, etal. PRB, 2007

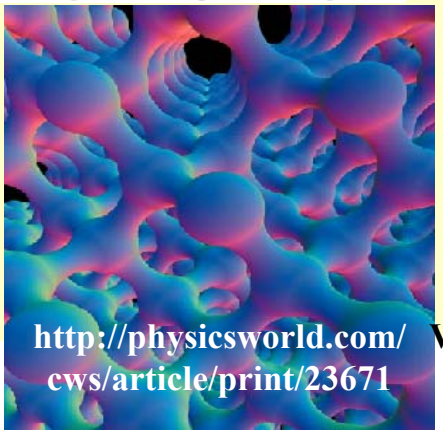


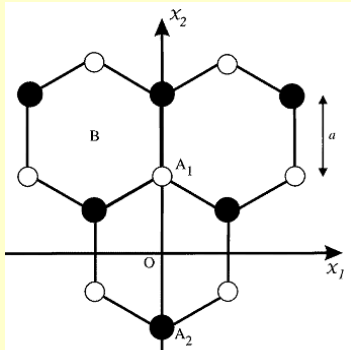
Bazan, etal. APL, 2007



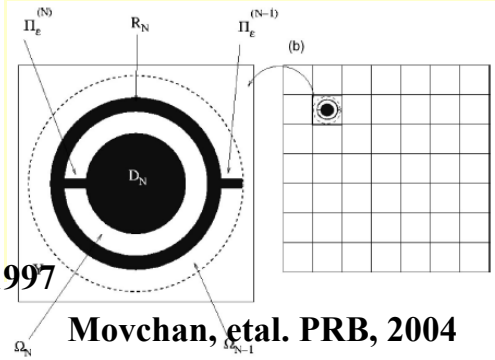
Ramprasad, etal. APL, 2005



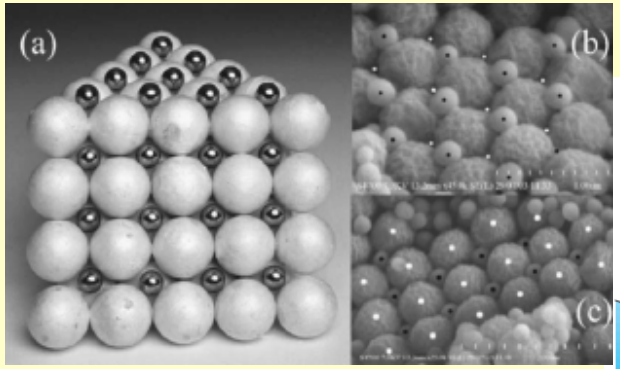




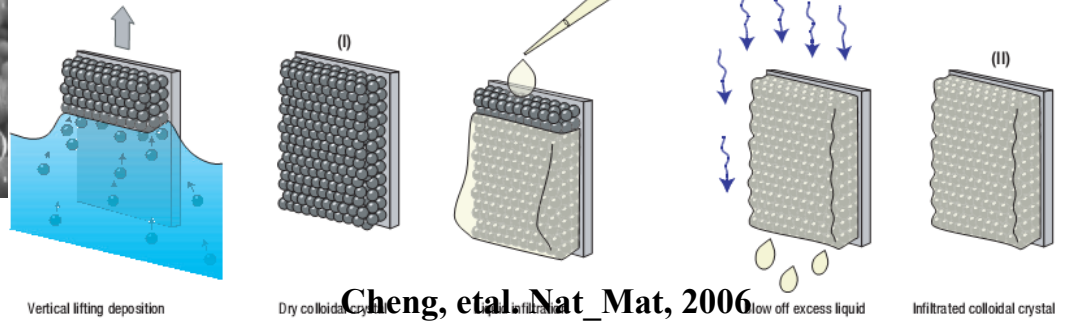
Vasseur, etal. JP: CM, 1997



Movchan, etal. PRB, 2004



Tommaseo, etal. JCP, 2007



Cheng, etal. Nat_Mat, 2006

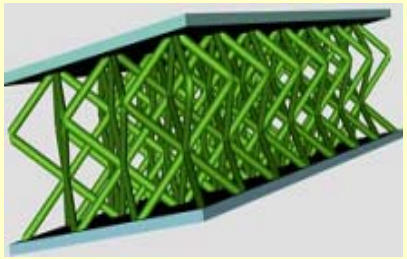


Hu, etal. PRE, 2005

概念的拓展

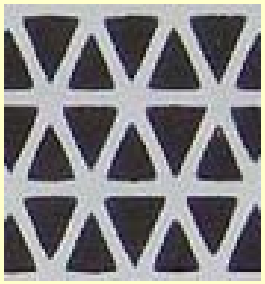
点阵/格栅材料

甄妮等, 力学学报, 2008

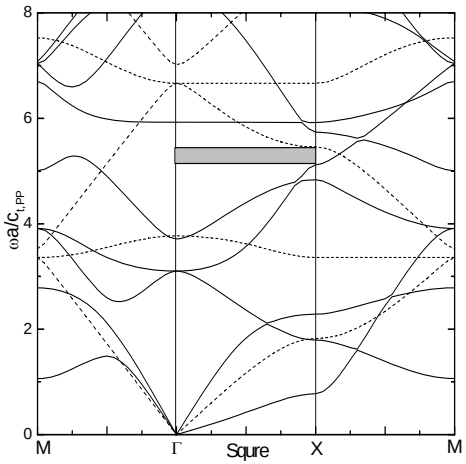


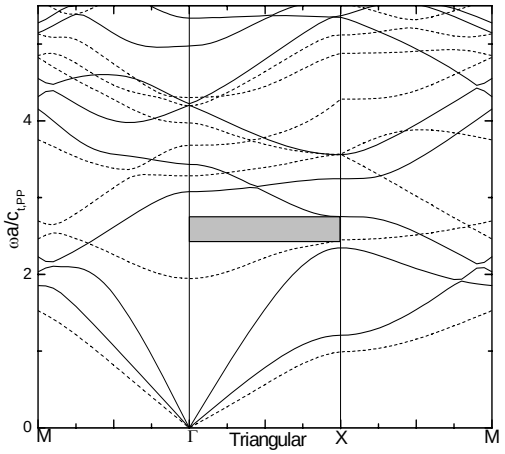
Al

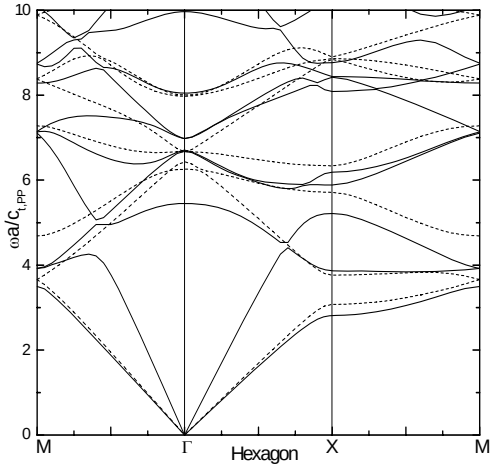


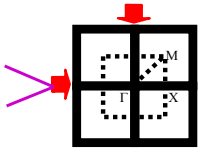


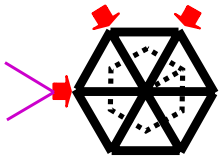
PP



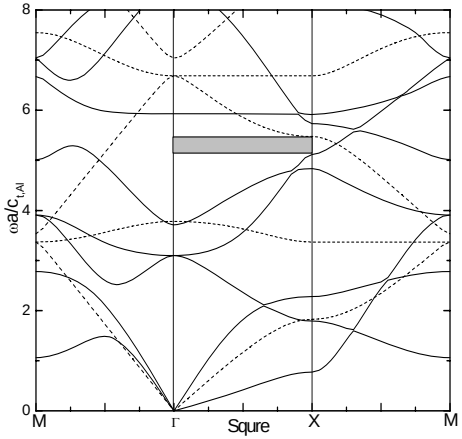


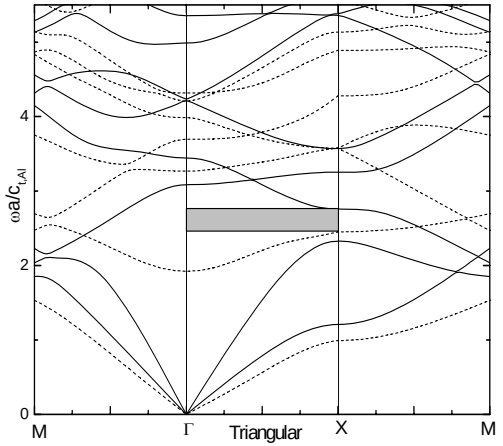


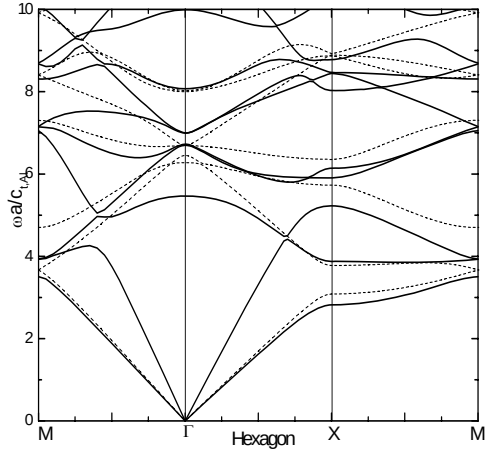






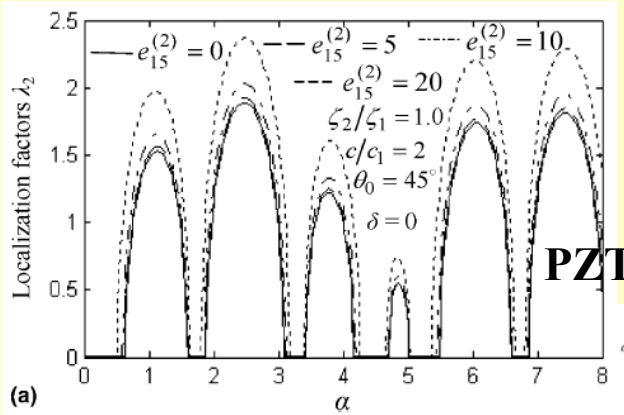




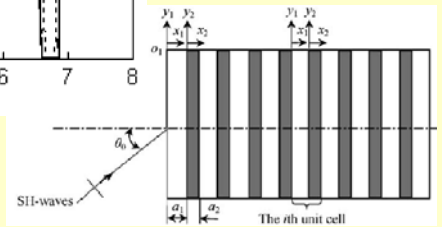


带隙调控-14

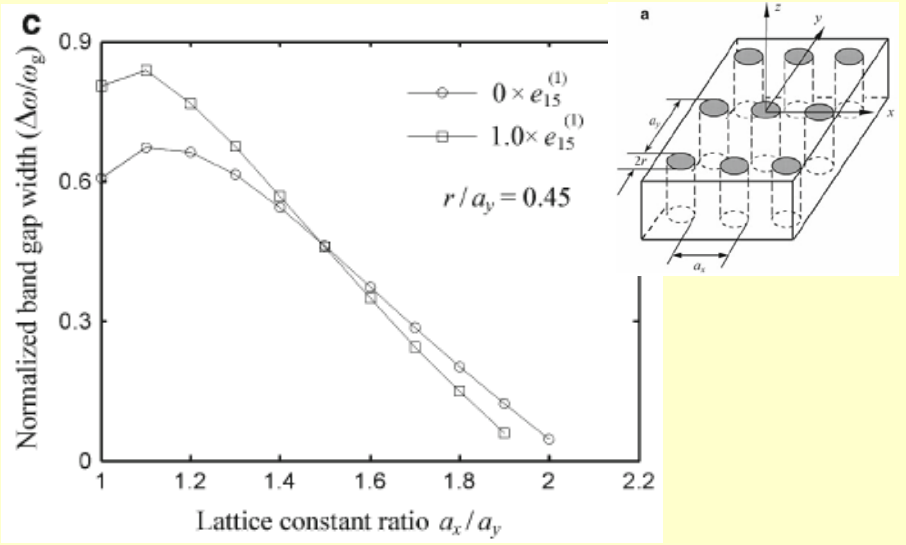
压电/压磁材料



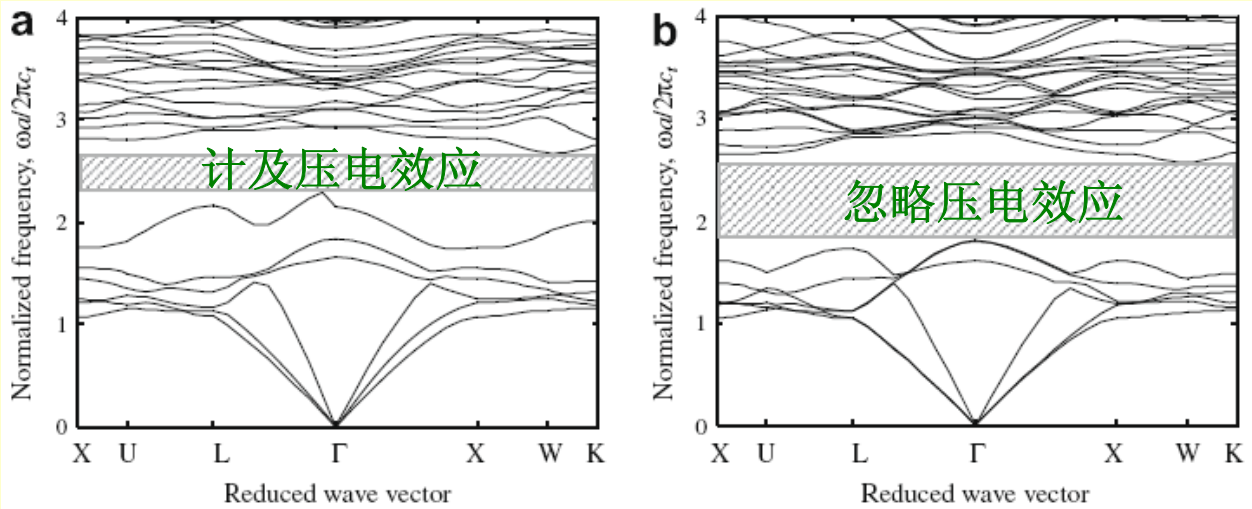
PZT5H/Polythene



Li, Wang, IJSS, 2005



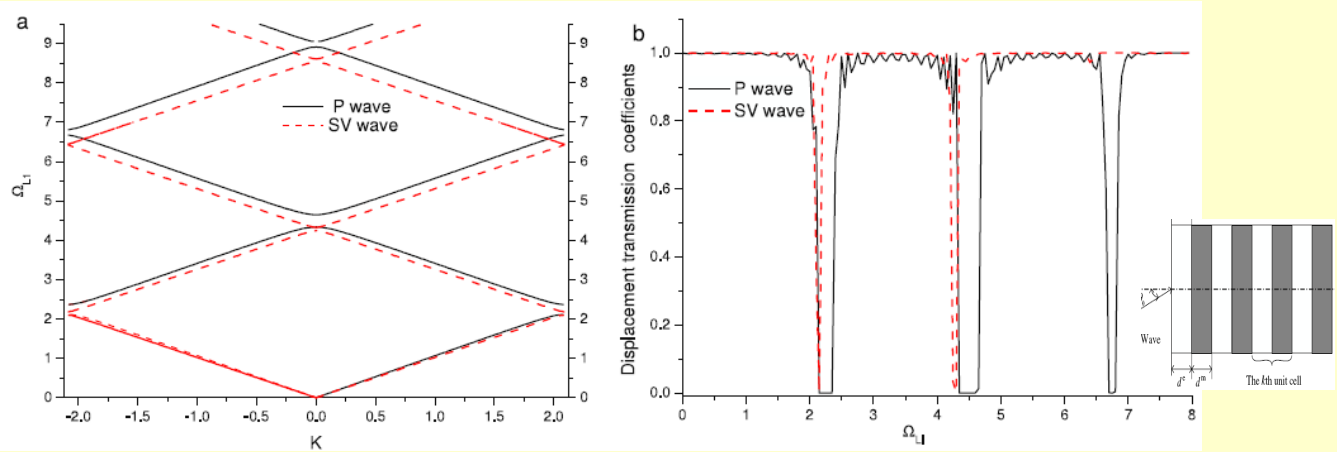
Wang et al, AMS, 2009 (PZT4/Polymer)

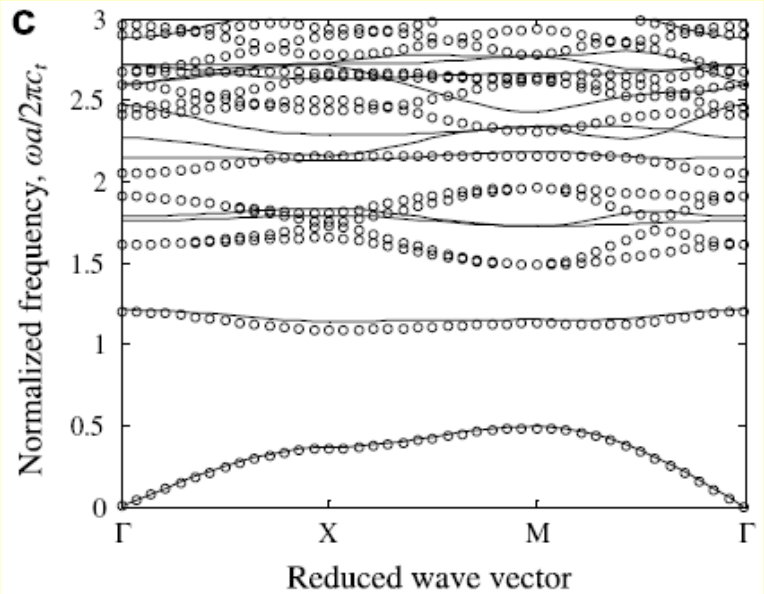


Wang et al, MRC, 2009
($BaTiO_3$/Polymer)

压电/压磁材料

Pang, SMS, 2010
($BaTiO_3/CoFe_2O_4$)



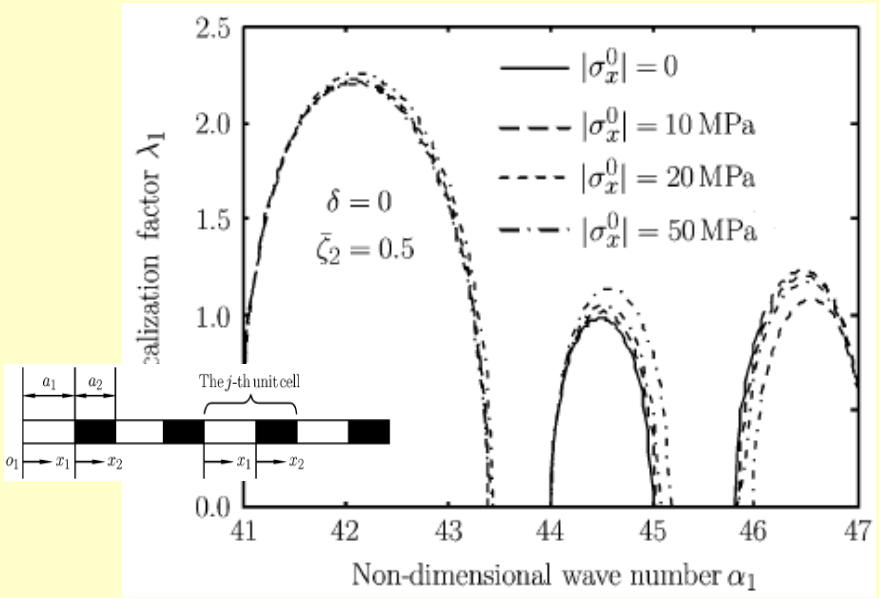


Wang et al, IJSS, 2008
($BaTiO_3$-$CoFe_2O_4$/Polymer)

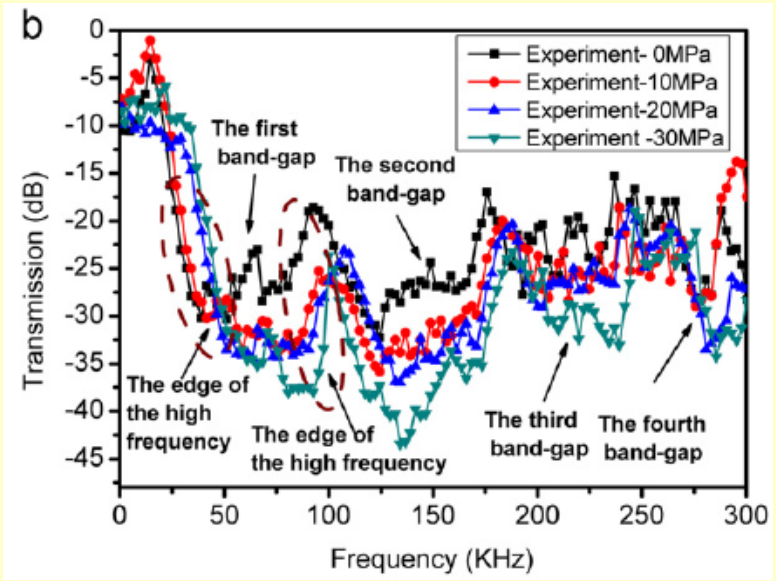
实线：计及压电/压磁效应

圆点：忽略压电/压磁效应

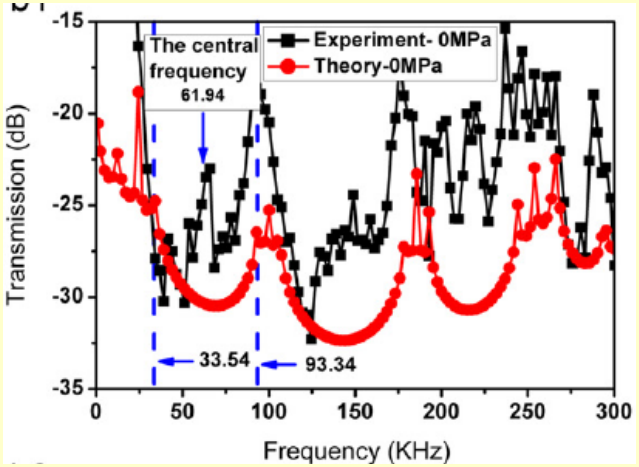
初始应力的影响

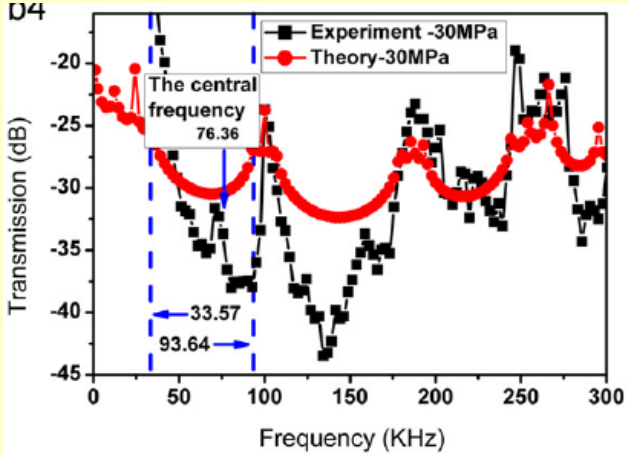


Wang et al, AMSS, 2008 (PZT/Epoxy)



Feng et al, PhysB, 2012 (Al/Epoxy)

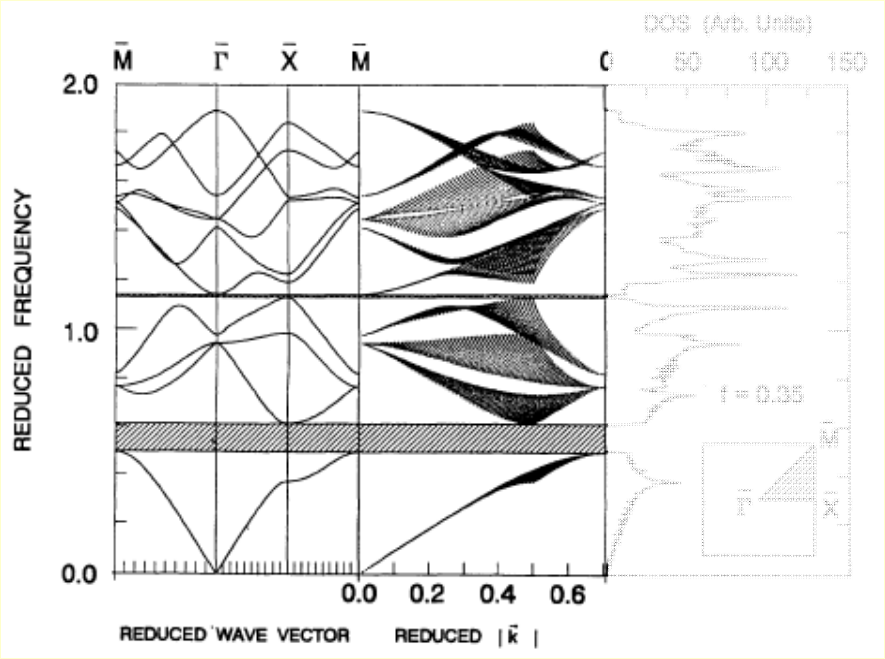


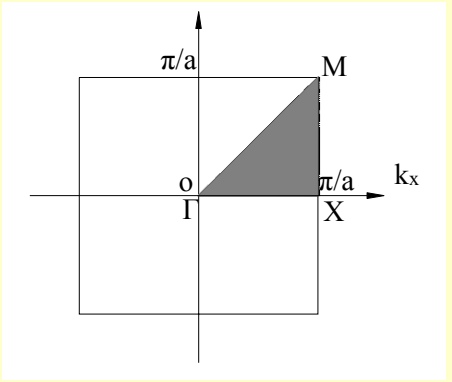


声学特征的表征参数-1

(1) 能带结构(频散关系)

- $\omega \sim \mathbf{k}$ 关系
- 由Brillouin区的高对称边界⇒ 完全或方向带隙
- 适用于周期系统





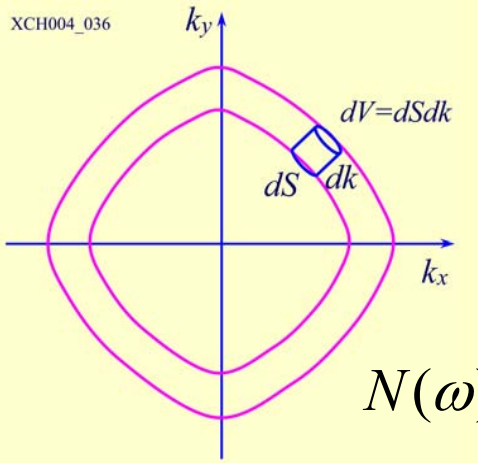
Kushwaha, et al. PRB, 1994 (Ni/Al)

声学特征的表征参数-2

(2) 态密度 (DOS)

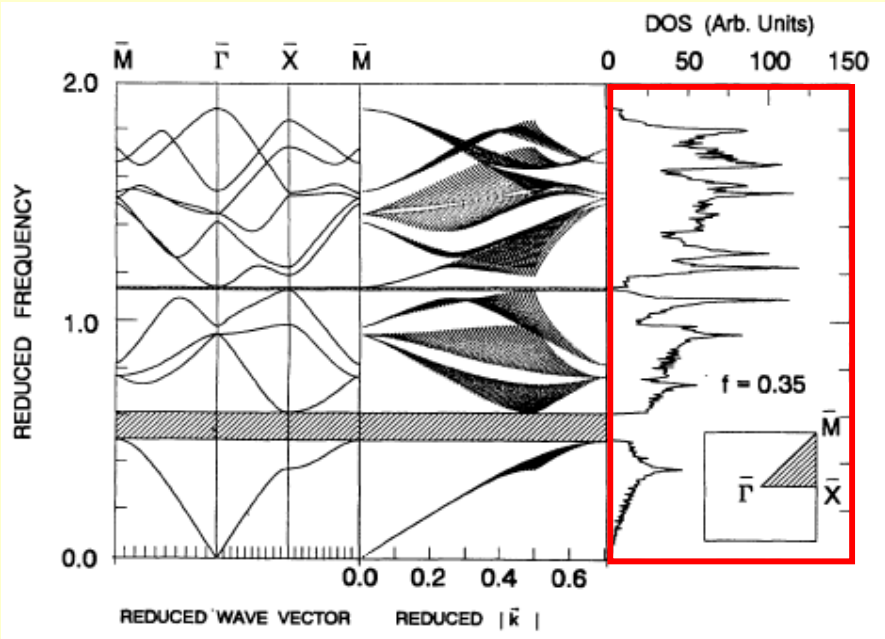
— 单位频率间隔内态的数量

$$N(\omega) = \lim_{\Delta\omega \to 0} \frac{\Delta k}{\Delta \omega}$$



iso-frequency surface

$$N(\omega) = \frac{\omega}{(2\pi)^3} \int \frac{dS}{|\nabla_k \omega|}$$



Kushwaha, et al. PRB, 1994 (Ni/Al)

- 适用于周期/非周期系统
- 不适宜方向带隙

声学特征的表征参数-3

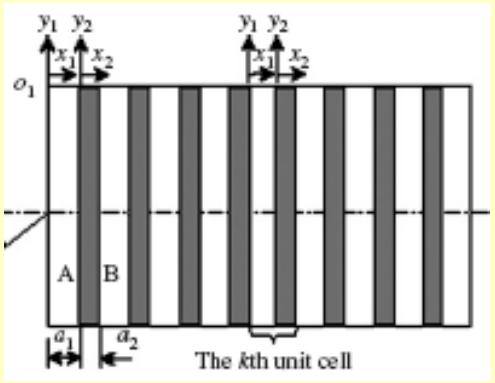
(3) 局部化长度 (局部化因子)

传播衰减: $e^{-x/l}$ or $e^{-n\lambda}$

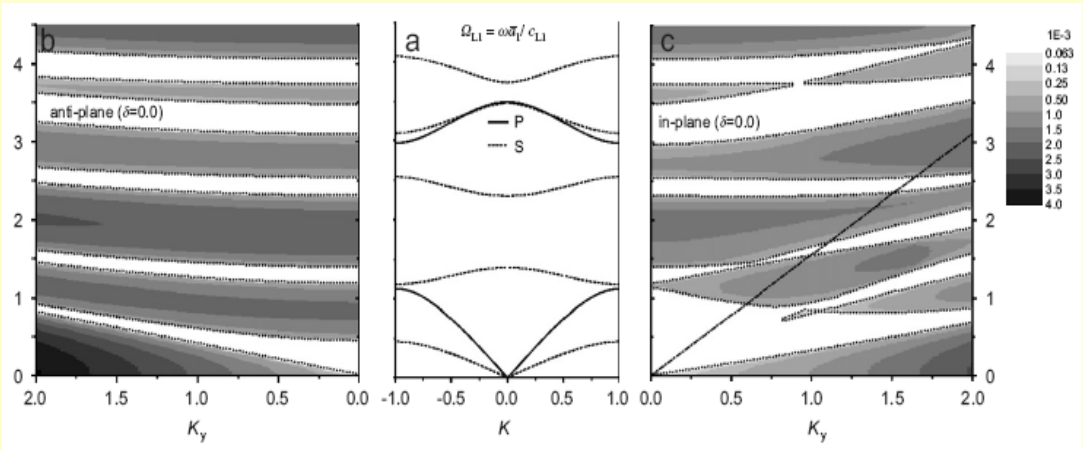
n*— 单元数, *n=x/a

λ — 局部化因子 ($\Leftrightarrow$ 最小Lyapunov指数)

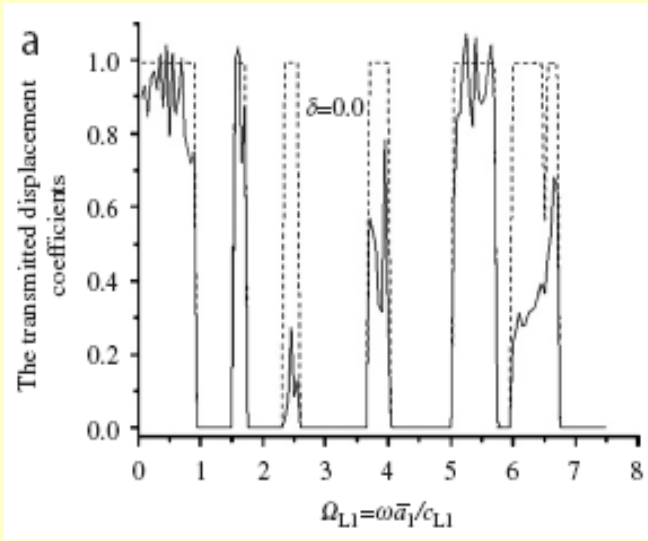
***l* — 局部化长度, *l* = *a*/ λ**



- **2或3维系统难以定义和计算**



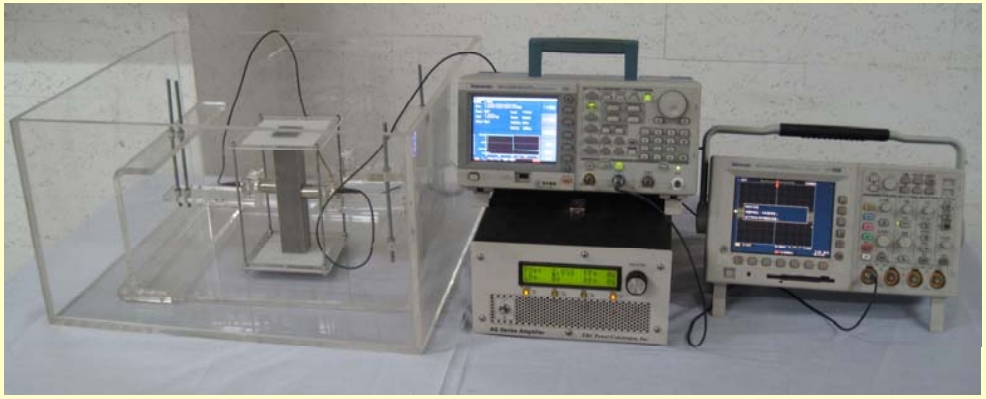
Chen, Wang, Phys.B, 2007



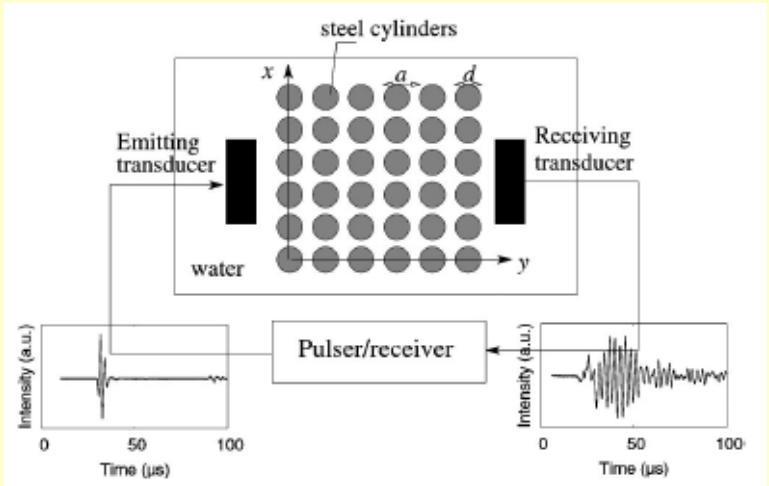
声学特征的表征参数-4

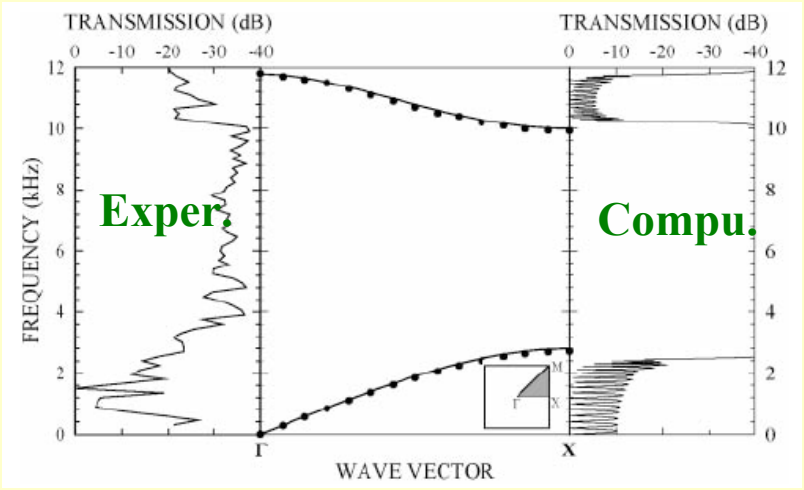
(4) 传输谱 (透射/反射)

- 数值计算
- 实验测量

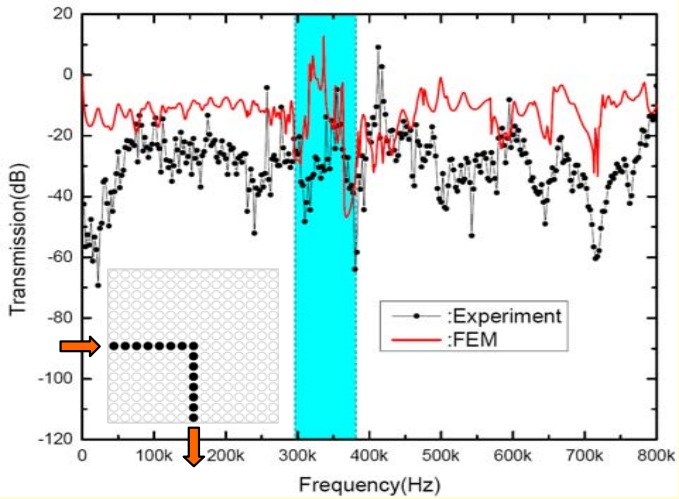


超声测量





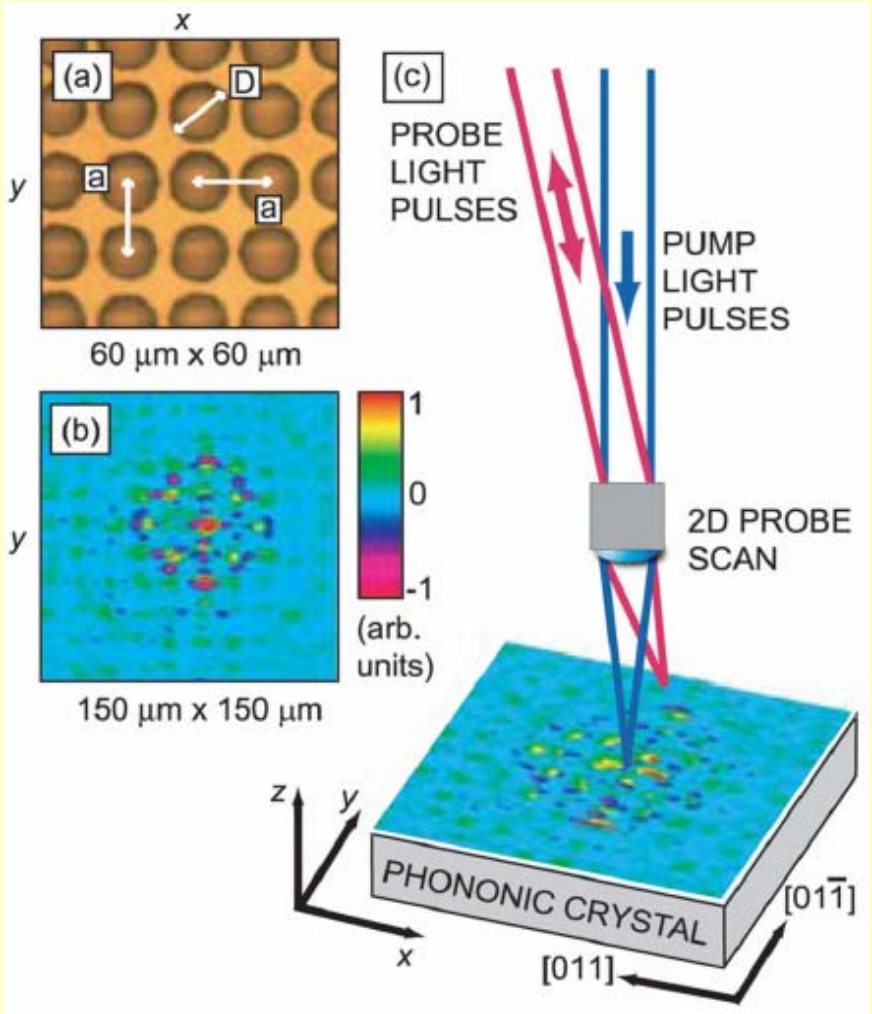
Vasseur, et al. Z. Kristallogr, 2005

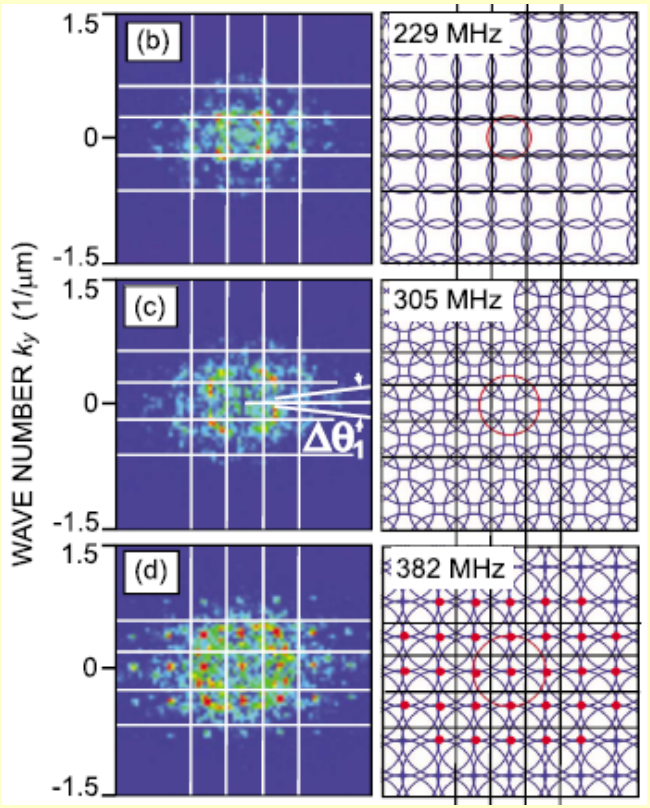


李建宝, 博士论文, 2011

声学特征的表征参数-5

光测，Dynamic visualization of surface acoustic waves





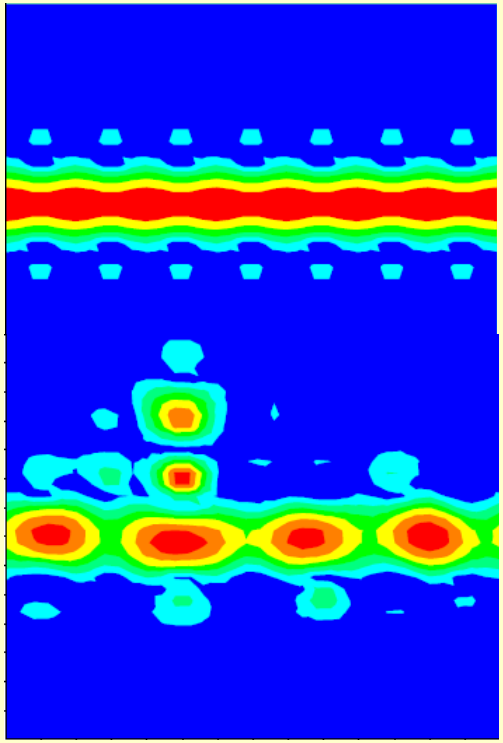
空气/硅 (40nm金覆层)

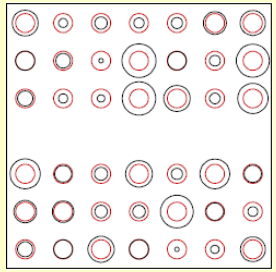
Profunse, et al. PRE, 2009

声学特征的表征参数-6

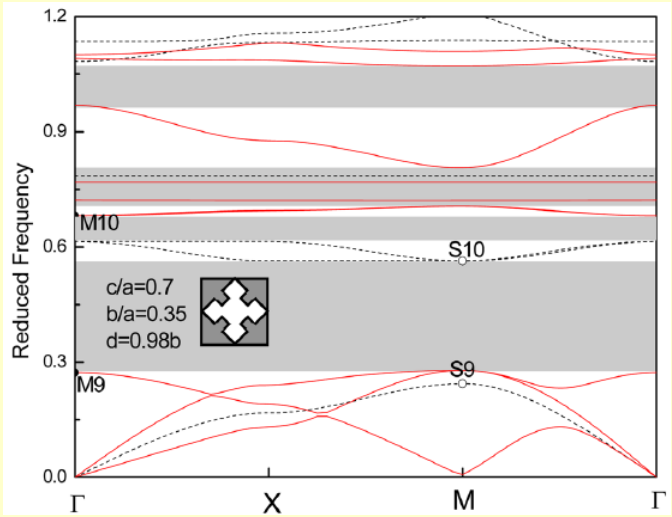
(5) 模态分布(波场强度分布)

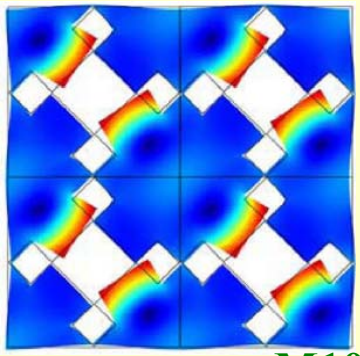
波场强度分布: **u, v, p, … ~ (*x*,*y*,*z*)**



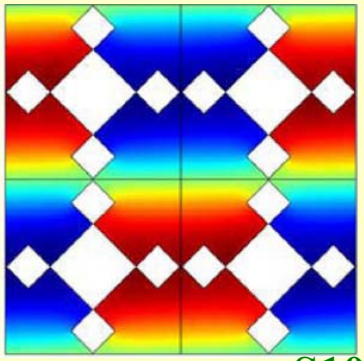


Chen, et al, AMR, 197-198, 2011





M10



S10

Wang, et al, JAP, 110, 2011

声子晶体的困难：

弹性波—矢量波

混合模态(耦合的纵横波、非耦合的横波)

纵横模态波速不同

固体-流体混合(弹性波-声波)

能带结构的数值计算方法

计算带结构的常用方法:

(1) 平面波展开法(PWE)***

(2) 小波函数展开法(Wavelet)*

(3) 柱面/球面波展开法**

—多散射法(MST)、DtN映射法

(4) 传递矩阵法(TMM)***

[离散方法]

(5) 有限差分法(FDTD)***

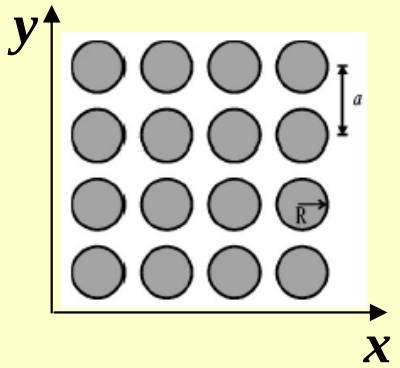
(6) 有限元法(FEM)***

(7) 边界元法(BEM)*

(8) 集中质量法(LMM)*

(1) 平面波展开法(PWE)

基于Fourier分析的方法



$$\mathbf{r} = (x, y, z)$$

$$\mathbf{u}(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{u}_{\mathbf{k}}(\mathbf{r}) \qquad \textbf{(Bloch theorem)}$$

$$(\nabla + i\mathbf{k})\cdot[\mathbb{C} : (\nabla + i\mathbf{k}) \otimes \mathbf{u}_{\mathbf{k}}(\mathbf{r})] = -\rho(\mathbf{x})\omega^2\mathbf{u}_{\mathbf{k}}(\mathbf{r})$$

$$\mathbf{u}_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \hat{\mathbf{u}}_{\mathbf{k}}(\mathbf{G})\mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}}$$

$$\{\rho, \mathbb{C}\}(\mathbf{r}) = \sum_{\mathbf{G}} \{\hat{\rho}, \hat{\mathbb{C}}\}(\mathbf{G})\mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}}$$

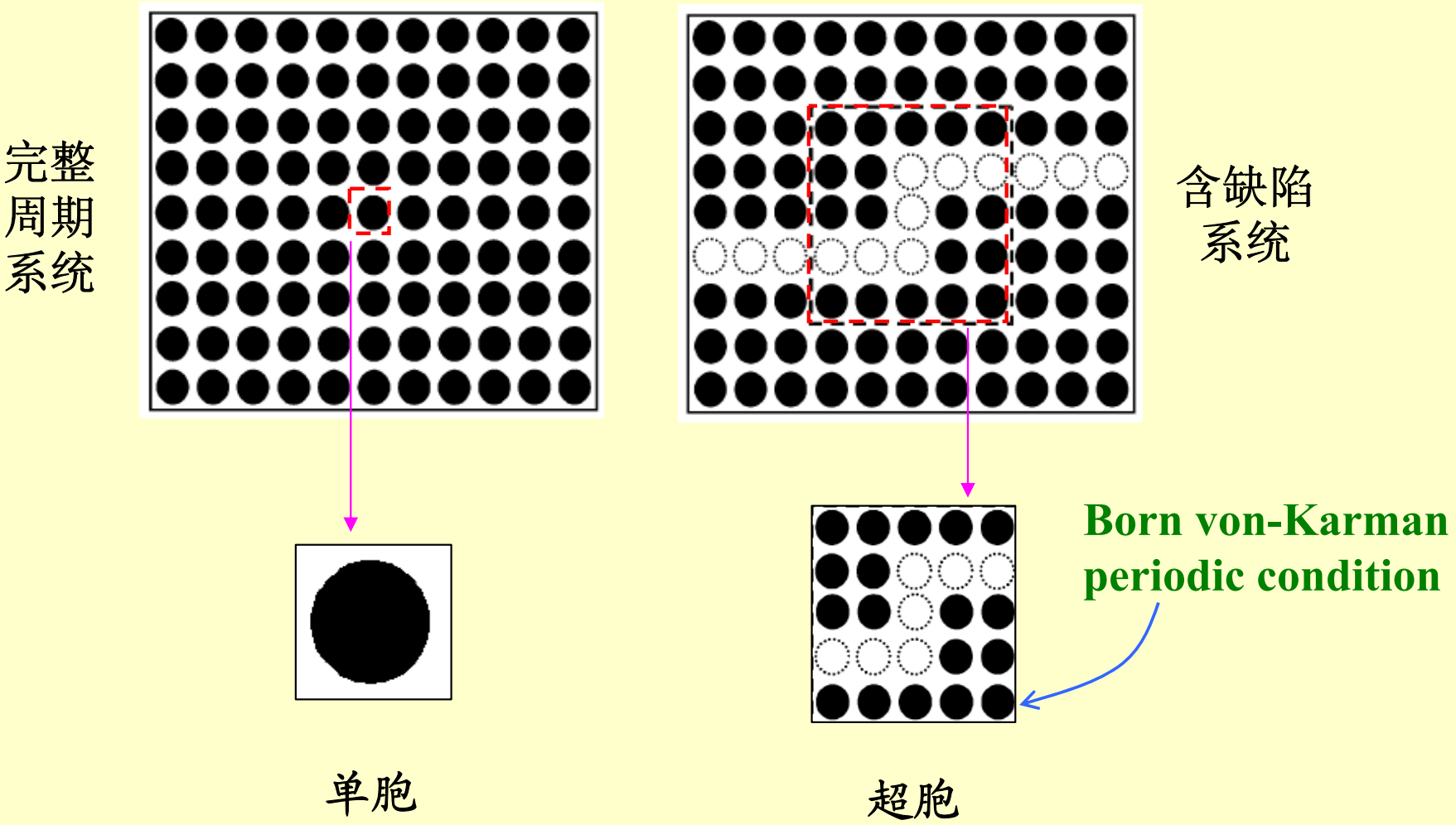
(Fourier expansion)

$$\mathbf{M}\cdot\hat{\mathbf{u}}_{\mathbf{k}} = \omega^2\mathbf{N}\cdot\hat{\mathbf{u}}_{\mathbf{k}}$$

A standard eigenvalue problem

(1) 平面波展开法(PWE)

单胞 & 超胞



(1) 平面波展开法(PWE)

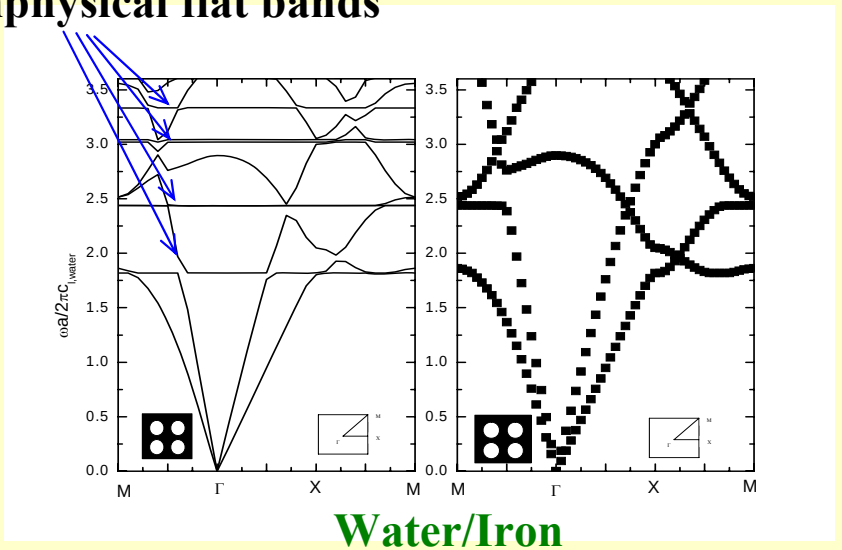
缺点：

- 因为满阵而计算时间长
- 因为Gibbs现象而收敛满
- 对流固混合体系收敛差/不适用
- 声学差异大或大的超胞收敛差
- 难以考虑界面连接的差异



Modified PWE method

unphysical flat bands



Water/Iron

(1) 平面波展开法(PWE)

修正的平面波展开法

— 基于Laurent逆定理

Laurent定理:

$$h(x) = f(x)g(x)$$

$$h_n = \sum_{m=-\infty}^{+\infty} f_{n-m} g_m \qquad h_n = \sum_{m=-M}^{M} f_{n-m} g_m$$

Laurent逆定理:

若 ***f*(*x*)** 和 ***g*(*x*)** 在某点具有“互补间断”, 则该点为***h*(*x*)**的可去间断点， 于是

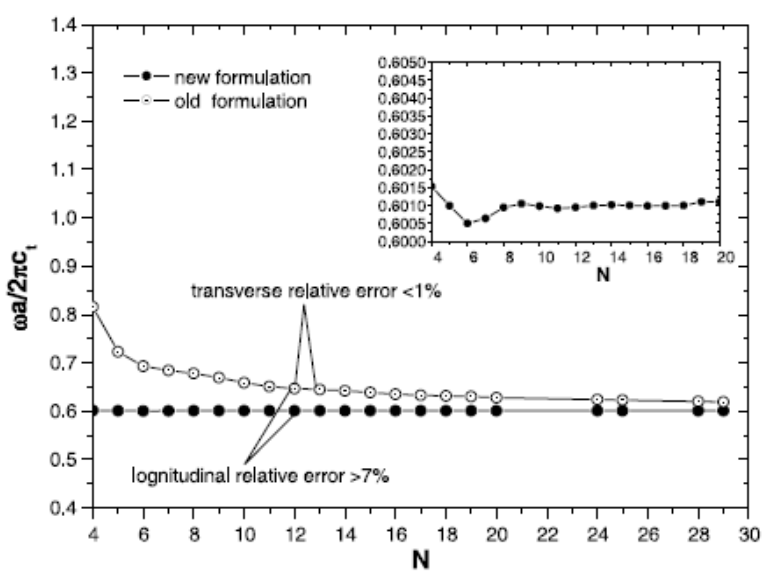
$$h_n = \sum_{m=-M}^{M} \left[1/f\right]^{-1}_{n-m} g_m$$

[1/*f*] is Toeplitz matrix

(1) 平面波展开法(PWE)

$$C_{ijkl}(\mathbf{x})\frac{\partial u_m(\mathbf{x})}{\partial x_n} \qquad (*) \text{—“stress”}$$

在界面上面力连续 → 上述量有些具有可去间断点。



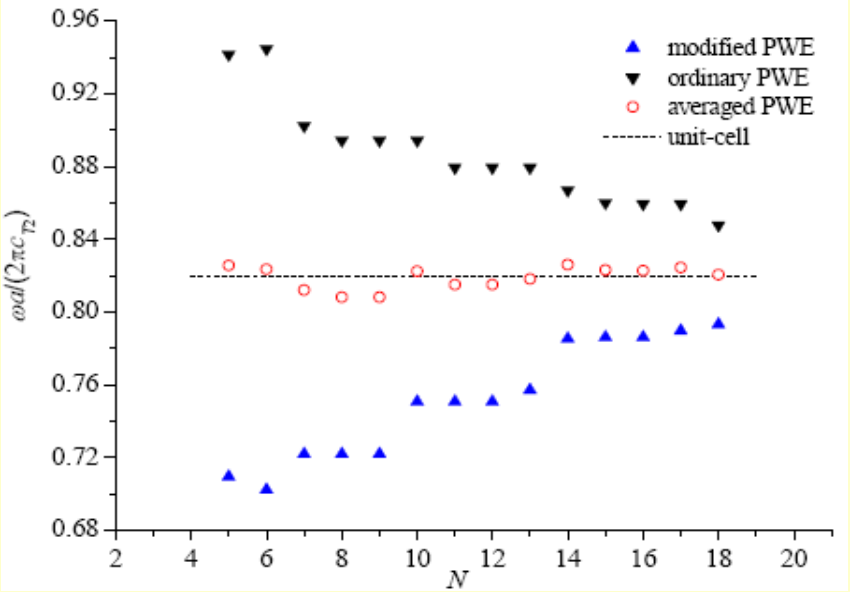
根据Laurent逆定理以 $[1/C_{ijkl}]^{-1}$ 代替 C_{ijkl}。

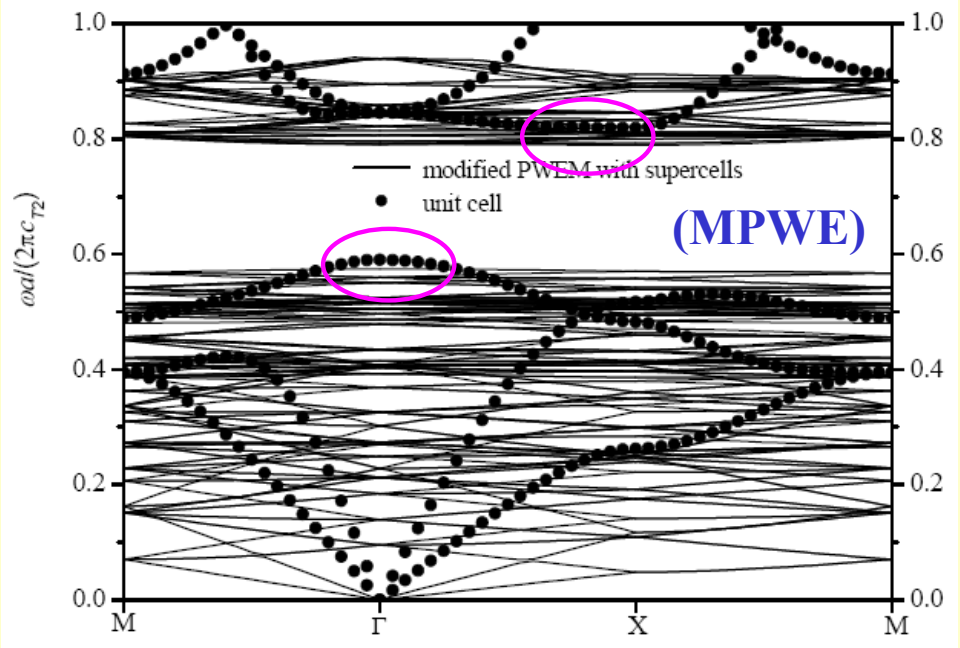
Cao et al. PLA, 2004 (Steel/Epoxy)

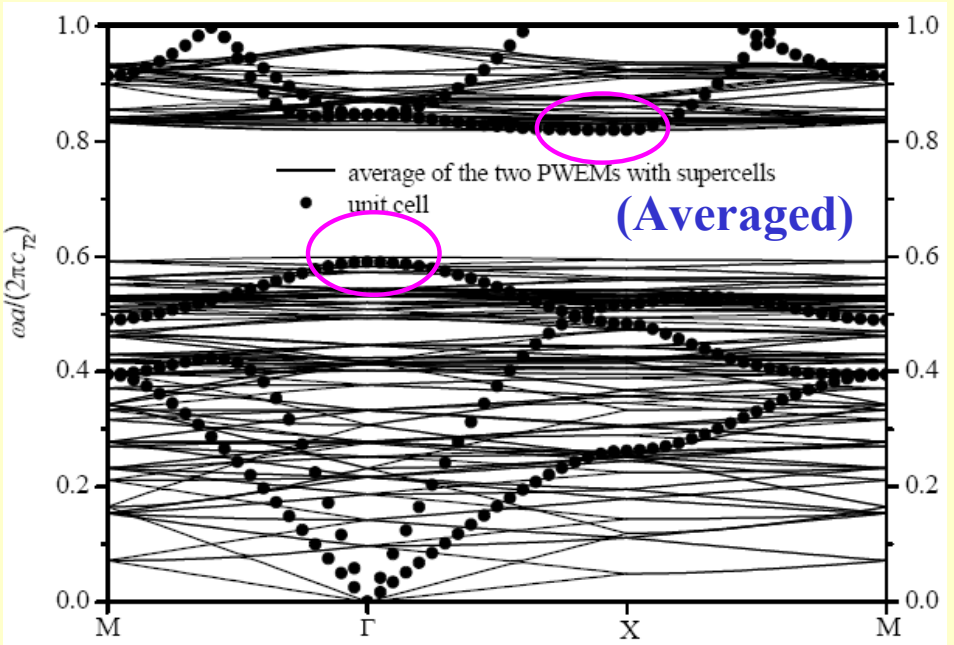
(1) 平面波展开法(PWE)

对大的超胞或声学差异大的系统结果仍然不精确！

Chen, PhD D., 2008; Chen, Wang, et al., WRCM, 2009 (Pb/Epoxy, 单胞 & 7×7 超胞)







(2) 小波函数展开法(Wavelet)

基于小波分析理论的方法

Fourier 基函数

⇒ 小波基函数

(局域性, 震荡性, 多层结构...)

Details:

Yan & Wang, Sci. in China G, 2007 for 1D bulk waves

Yan & Wang, PRB, 2006 for 2D bulk waves

Yan & Wang, PRB, 2008 for 2D surface waves

Yan, Wang & Zhang, AMSS, 2008 for defect modes (BW)

(2) 小波函数展开法(Wavelet)

周期函数的周期小波展开:

1 D:

$$f(x)=\underbrace{\sum_{k=0}^{2^{j_0}-1} s_k \varphi_{j_0,k}^{period}(x)}_{\text{wavelet series at } j_0 \text{ scale}}+\underbrace{\sum_{\substack{j\in Z\\ j\geq j_0}}\sum_{k=0}^{2^{j}-1} d_{j,k}\psi_{j,k}^{period}(x)}_{\text{Complementary part at a finer scale}},\quad x\in[0,1]$$

φ：尺度函数;　　ψ：小波函数

2 D:

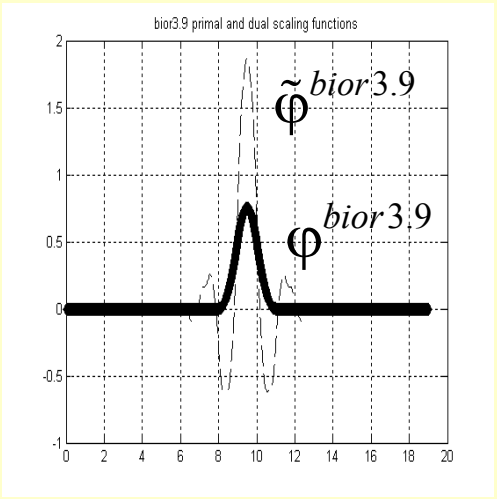
$$f(x,y)=\sum_{k1=0}^{2^{j0}-1}\sum_{k2=0}^{2^{j0}-1}\chi_{k1,k2}\varphi_{j_0,k1,k2}^{period}(x,y)+\sum_{\substack{j\in Z\\ j\geq j_0}}\sum_{k1=0}^{2^{j}-1}\sum_{k2=0}^{2^{j}-1}\gamma_{j,k1,k2}\psi_{j,k1,k2}^{(\lambda)\,period}(x,y),$$

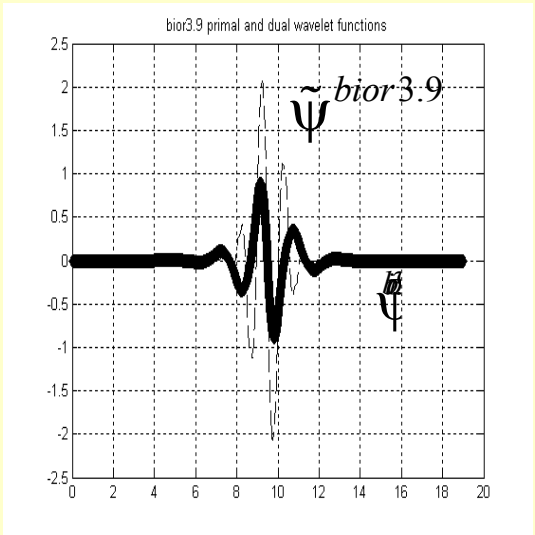
$$\lambda=1,2,3,\ x,y\in[0,1]$$

(2) 小波函数展开法(Wavelet)

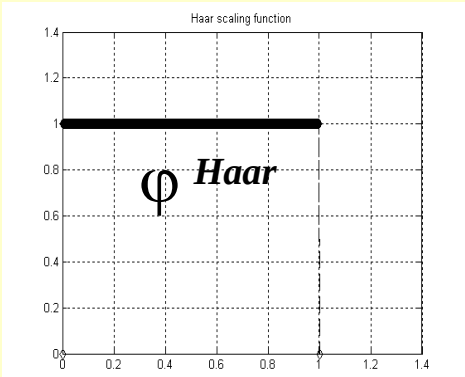
材料参量(间断) — **Haar wavelets**

位移场 — **Bior3.9 wavelets**

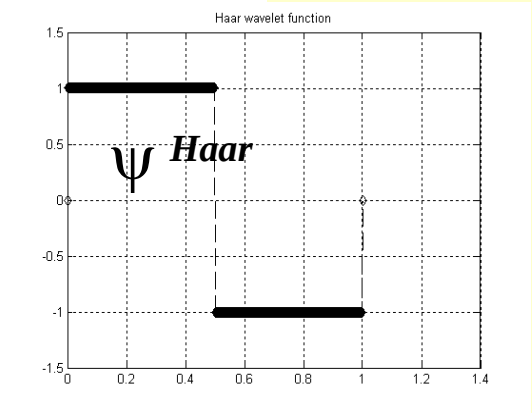




2 D



1 D



$$\varphi(x,y)=\varphi(x)\varphi(y) \qquad \psi^{(1)}(x,y)=\varphi(x)\psi(y)$$

$$\psi^{(2)}(x,y)=\psi(x)\varphi(y) \qquad \psi^{(3)}(x,y)=\psi(x)\psi(y)$$

(2) 小波函数展开法(Wavelet)

$$(\nabla + i\mathbf{k}) \cdot [\mathbb{C} : (\nabla + i\mathbf{k}) \otimes \mathbf{u}_\mathbf{k}(\mathbf{r})] = -\rho(\mathbf{r})\omega^2 \mathbf{u}_\mathbf{k}(\mathbf{r})$$

变分形式:

$$\left\langle v,\ (\nabla + i\mathbf{k}) \cdot [\mathbb{C} : (\nabla + i\mathbf{k}) \otimes \mathbf{u}_\mathbf{k}(\mathbf{r})] \right\rangle = -\omega^2 \left\langle v,\ \rho(\mathbf{r})\mathbf{u}_\mathbf{k}(\mathbf{r}) \right\rangle$$

or

$$\int_\Omega \mathbb{C} : (\nabla + i\mathbf{k}) \otimes \mathbf{u}_\mathbf{k}(\mathbf{r}) \cdot \overline{(\nabla + i\mathbf{k})v} d\mathbf{r} = \omega^2 \int_\Omega \rho(\mathbf{r})\mathbf{u}_\mathbf{k}(\mathbf{r})\bar{v} d\mathbf{r}$$

$\boldsymbol{v}$ — 任意平方可积函数

小波展开:

$$\mathbf{u}_\mathbf{k}(\mathbf{r}) = \sum_{b_m \in \Psi_{j_0,J}} \hat{\mathbf{u}}_{\mathbf{k},m} b_m$$

$v = b_q$ (小波基函数)

(2) 小波函数展开法(Wavelet)

$$\int_{\Omega} \mathbb{C} : [(\nabla + i\mathbf{k}) \otimes \hat{\mathbf{u}}_{\mathbf{k},p} b_p] \cdot \overline{(\nabla + i\mathbf{k}) \tilde{b}_q} d\mathbf{r} = \omega^2 \int_{\Omega} \rho(\mathbf{x}) \hat{\mathbf{u}}_{\mathbf{k},p} b_p \tilde{b}_q d\mathbf{r}$$

$$\boxed{\mathbf{M} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = \omega^2 \mathbf{B} \cdot \hat{\mathbf{u}}_{\mathbf{k}}}$$

$$(M)_{p,q} = \int_{\Omega} \mathbb{C} : [(\nabla + i\mathbf{k}) b_p] \cdot \overline{(\nabla + i\mathbf{k}) \tilde{b}_q} d\mathbf{r} \qquad (B)_{p,q} = \int_{\Omega} \rho(\mathbf{r}) b_p \tilde{b}_q d\mathbf{r}$$

$$(\rho(\mathbf{r}), \mathbb{C}(\mathbf{r})) = \sum_{d_m \in \Psi_{j_0,J}} (\hat{\rho}_{\mathbf{k},m}, \hat{\mathbb{C}}_{\mathbf{k},m}) d_m$$

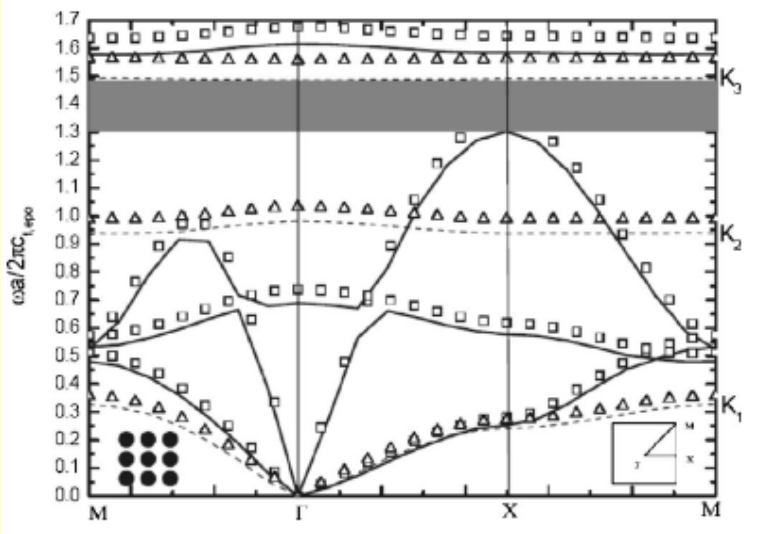
$$\int_{\Omega} \psi^{period,Haar}(\mathbf{r}) (\nabla + i\mathbf{k}) b_p \cdot \overline{(\nabla + i\mathbf{k}) \tilde{b}_q} d\mathbf{r}$$ — **Numerical evaluation**

Bertoluzza et.al. *ANM* (2000)

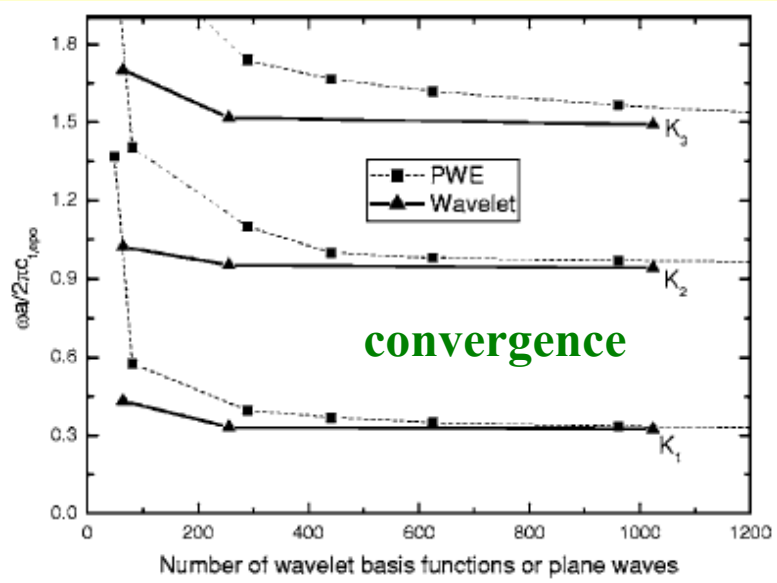
(2) 小波函数展开法(Wavelet)

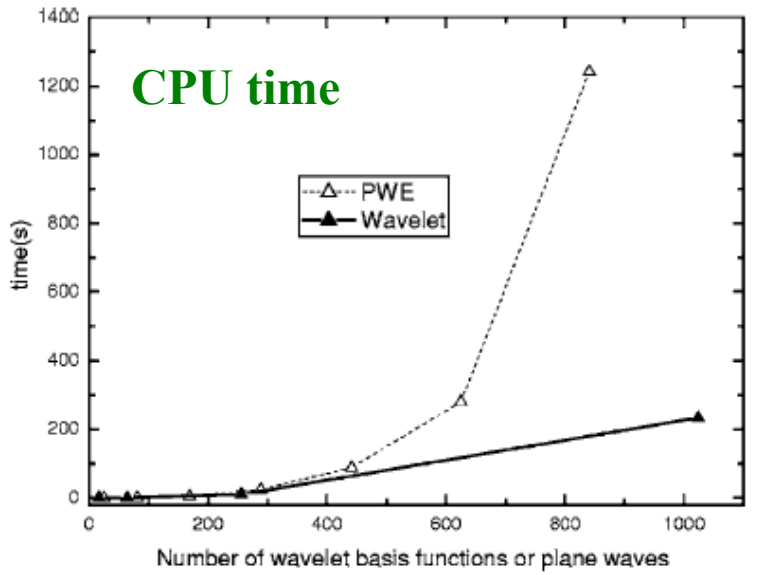
优点：

- 基函数选取的多样性
- 因稀疏矩阵而收敛快
- 计算速度快



Yan et al. PRB, 2006 (Au/Rubber)

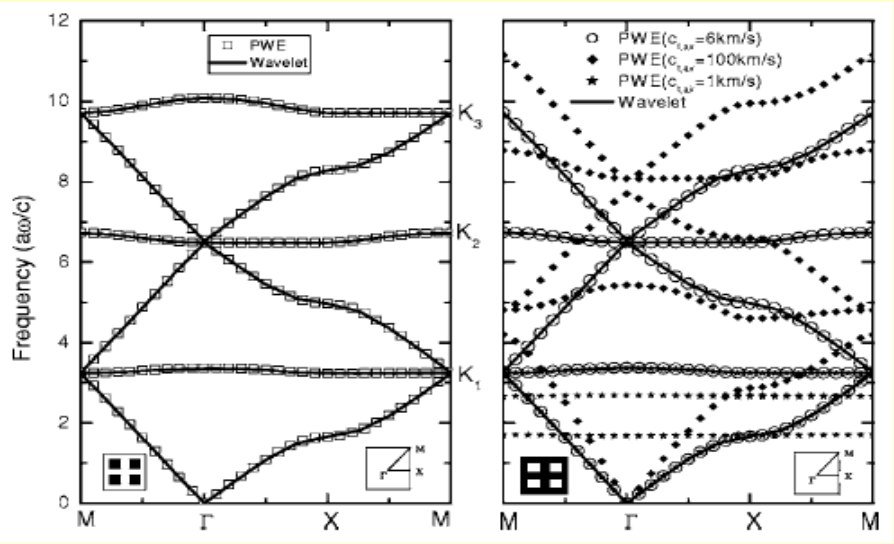




(2) 小波函数展开法(Wavelet)

- 适用于流固混合体系

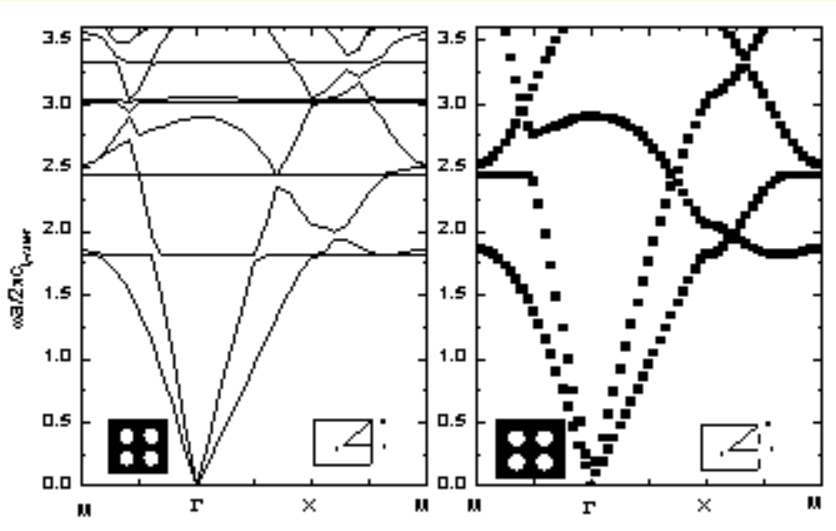
solid/fluid ⇒ "fluid"/fluid



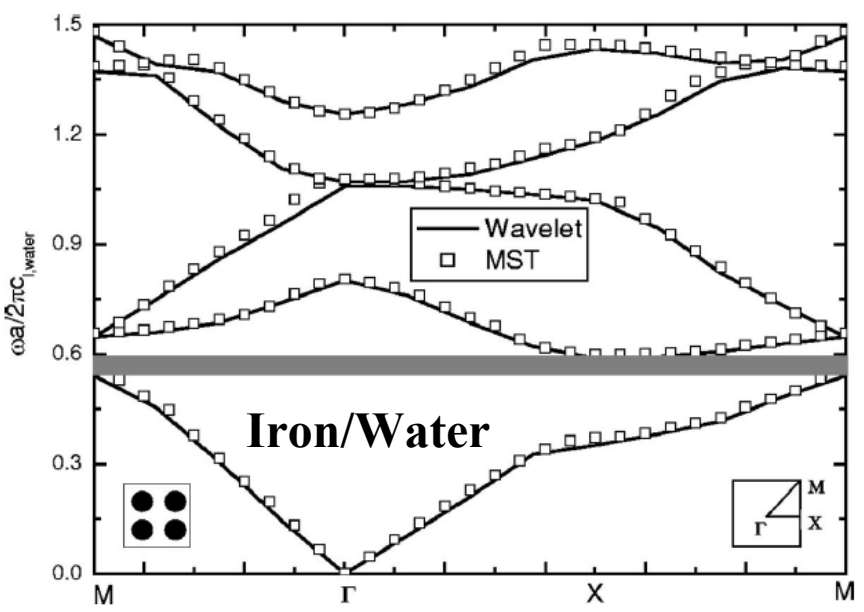
"Steel"/Air

Air/Steel

Yan et al. PRB, 2006

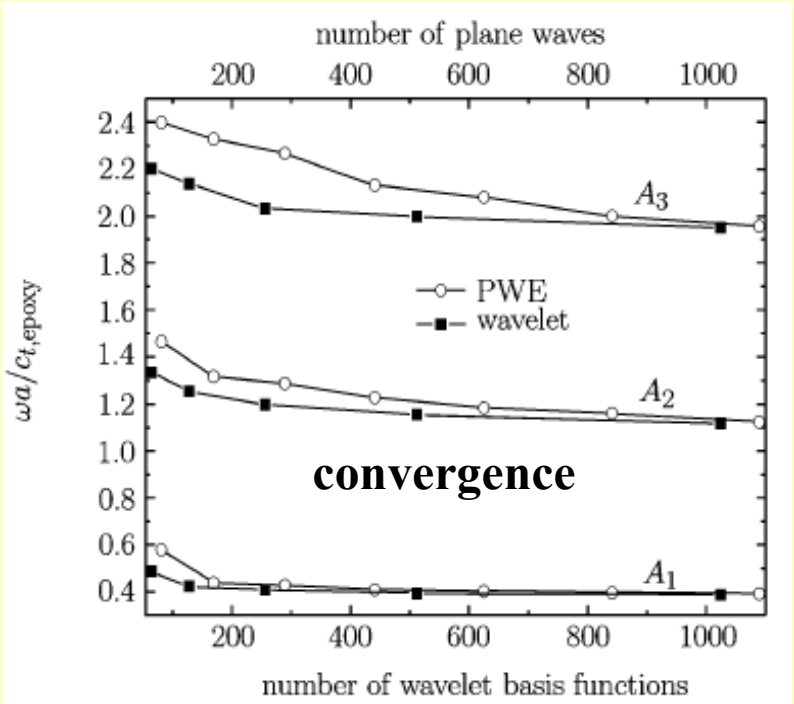


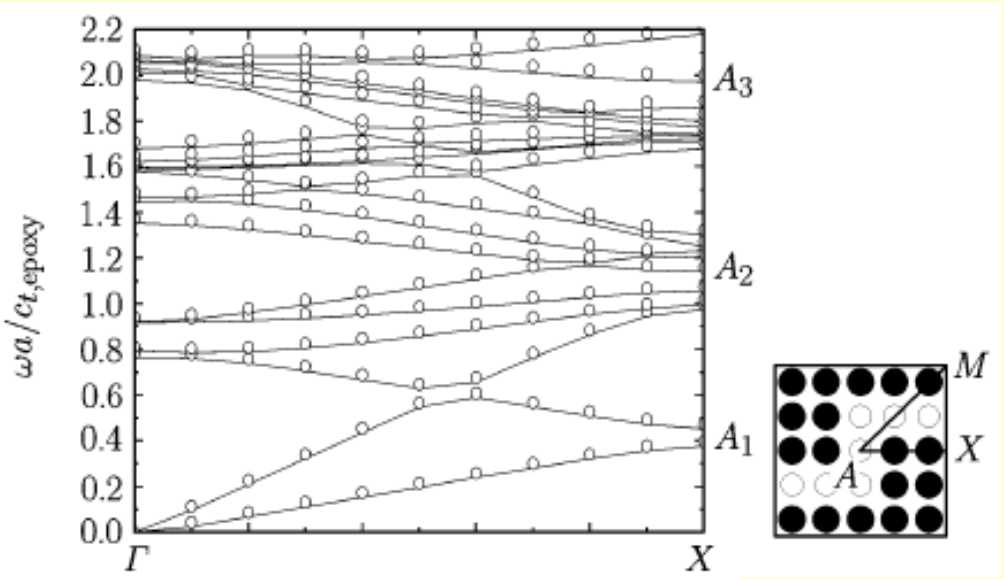
Water/Iron

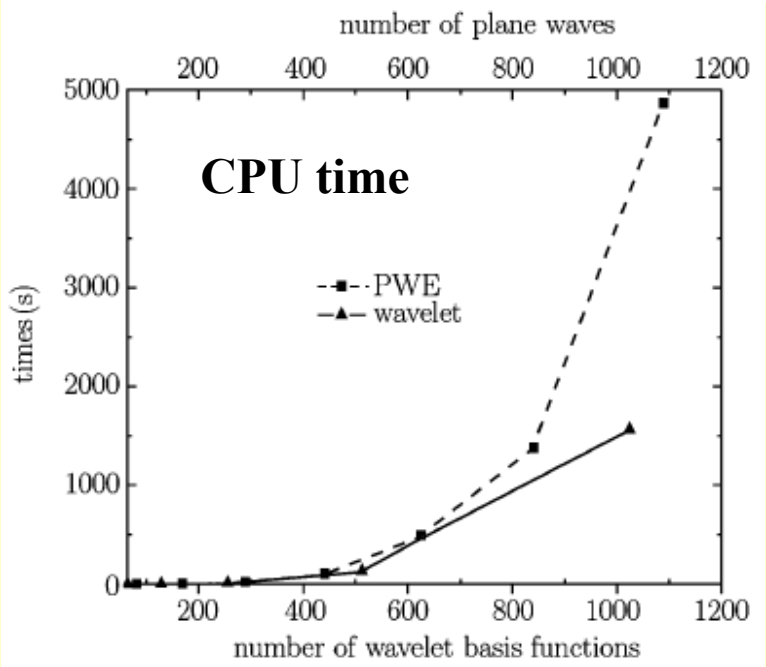


(2) 小波函数展开法(Wavelet)

- 适用于缺陷体系



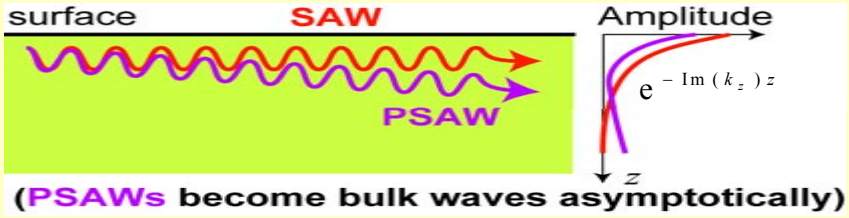


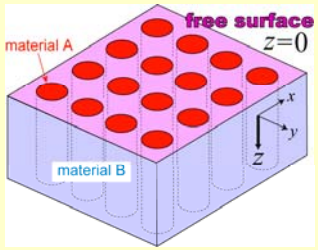


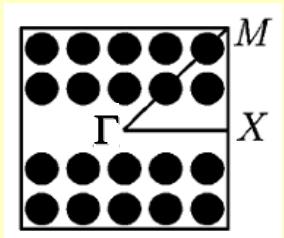
Yan et al.
AMSS, 2008
(Steel/Epoxy)

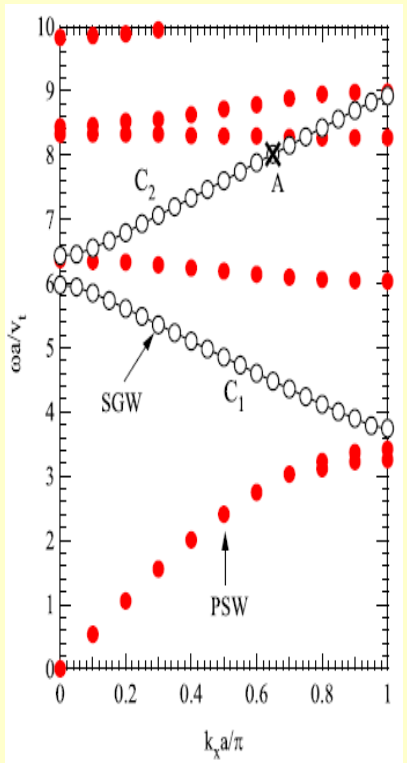
(2) 小波函数展开法(Wavelet)

- 适用于表面波

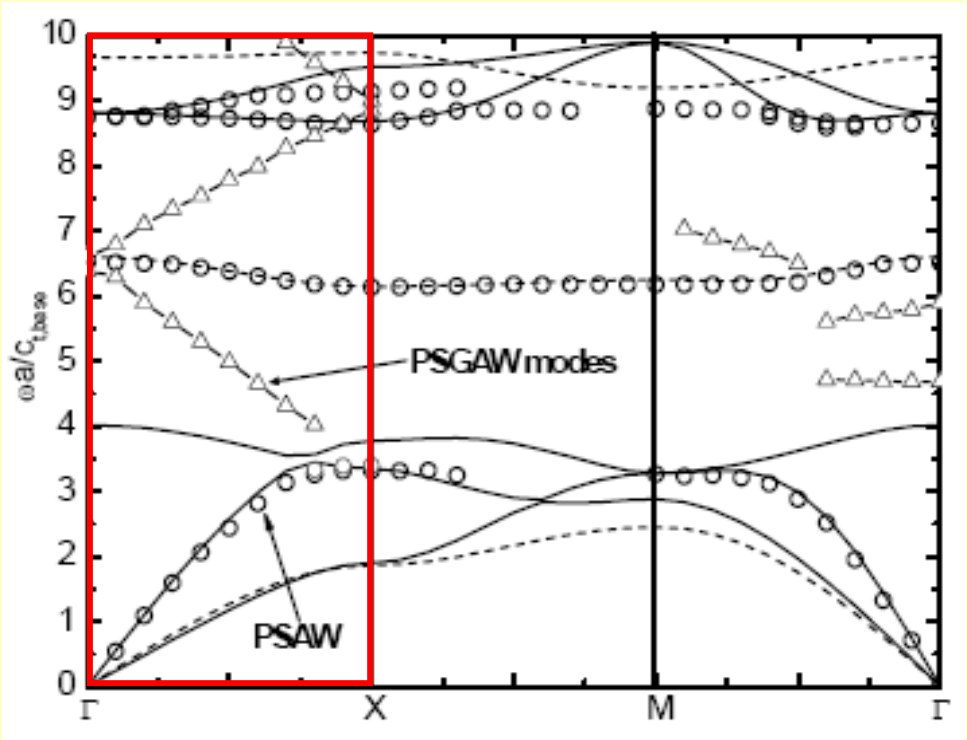








Tanaka et al. WMot, 2007 (FDTD)



Yan et al. PRB, 2008 (Steel/Epoxy)

(2) 小波函数展开法(Wavelet)

缺点：

- 数学非常复杂 (小波积分)
- 难以考虑界面连接的差异
- solid/fluid ⇒ “fluid”/fluid (高密度流体有问题)

(3) 柱/球波函数展开法-MST

多散射法（MST）

发展自量子力学**KKR**理论的方法

$$(\lambda+2\mu)\nabla(\nabla\cdot\mathbf{u})-\mu\nabla\times\nabla\times\mathbf{u}+\rho\omega^2\mathbf{u}=0$$

柱/球坐标系中的通解：

—柱面/球面波展开式

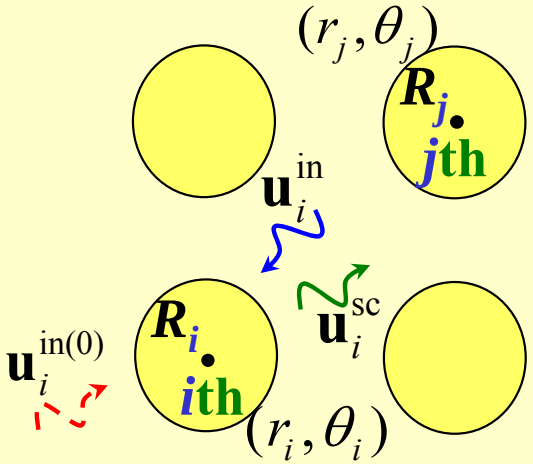
$$\mathbf{u}(\mathbf{r})=\sum_{n\sigma}[a_{n\sigma}\mathbf{j}_{n\sigma}(\mathbf{r})+b_{n\sigma}\mathbf{h}_{n\sigma}(\mathbf{r})]$$

$$(\mathbf{j}_{n\sigma},\mathbf{h}_{n\sigma})\sim \textit{cylindrical or spherical wave functions}$$

$$\sigma=1,2,3\sim \textit{P, SV, SH waves}$$

(3) 柱/球波函数展开法-MST

第 *i* 个散射体 (2D):



总散射场: $\mathbf{u}_i^{\text{sc}}(\mathbf{r}_i)=\sum_{n\sigma} b_{n\sigma}^i \mathbf{h}_{n\sigma}^i(\mathbf{r}_i)$

总入射场: $\mathbf{u}_i^{\text{in}}(\mathbf{r}_i)=\sum_{n\sigma} a_{n\sigma}^i \mathbf{j}_{n\sigma}^i(\mathbf{r}_i)$

$$\mathbf{r}_j=\mathbf{r}_i-(\mathbf{R}_j-\mathbf{R}_i)$$

外部散射场: $\mathbf{u}_i^{\text{in(0)}}(\mathbf{r}_i)=\sum_{n\sigma} a_{n\sigma}^{i(0)} \mathbf{j}_{n\sigma}^i(\mathbf{r}_i)$

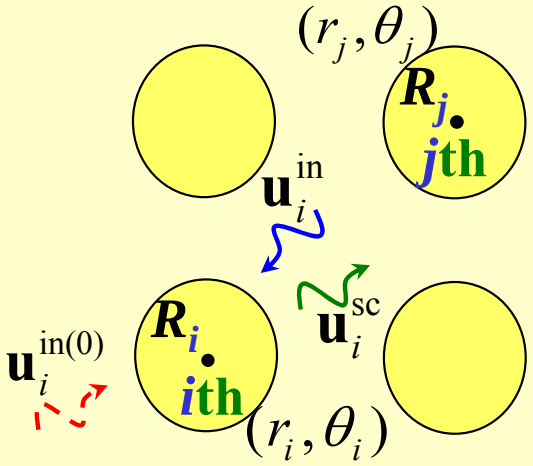
内部散射场: $\sum_{j\neq i}\sum_{n'\sigma'} b_{n'\sigma'}^j \mathbf{h}_{n'\sigma'}^j(\mathbf{r}_j)=\mathbf{u}_i^{\text{in}}(\mathbf{r}_i)-\mathbf{u}_i^{\text{in(0)}}(\mathbf{r}_i)$

$b_{n\sigma}^i=\sum_{n'\sigma'} t_{n\sigma n'\sigma'}^i a_{n'\sigma'}^i$ $\qquad \mathbf{T}^i=\{t_{n\sigma n'\sigma'}^i\}$: **Mie scattering matrix**

(3) 柱/球波函数展开法-MST

$$\sum_{jn'\sigma'}(\delta_{ij}\delta_{nn'}\delta_{\sigma\sigma'}-\sum_{n''\sigma''}G^{ij}_{n\sigma n''\sigma''}t^{j}_{n''\sigma''n'\sigma'})a^{j}_{n'\sigma'}=a^{i(0)}_{n\sigma}$$

(vector structure constant)



特征模态:

$$\det\left|\delta_{ij}\delta_{nn'}\delta_{\sigma\sigma'}-\sum_{n''\sigma''}G^{ij}_{n\sigma n''\sigma''}t^{j}_{n''\sigma''n'\sigma'}\right|=0$$

周期系统:

$$\mathbf{r}_j=\mathbf{r}_i-(\mathbf{R}_j-\mathbf{R}_i)$$

$$\det\left|\delta_{ss'}\delta_{nn'}\delta_{\sigma\sigma'}-\sum_{n''\sigma''}G^{ss'}_{n\sigma n''\sigma''}(\mathbf{k})t^{s'}_{n''\sigma''n'\sigma'}\right|=0$$

⇒ 能带结构

$$G^{ss'}_{n\sigma n''\sigma''}(\mathbf{k})=\sum_{\mathbf{R}}G_{n\sigma n''\sigma''}(\mathbf{o}_{s'}-\mathbf{o}_s+\mathbf{R})\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}}$$

(3) 柱/球波函数展开法-MST

优点:

- 可以计算能带、响应（层多散射法）
- 适用于流固混合系统
- 对3维系统易于实施
- 可考虑界面连接的差异

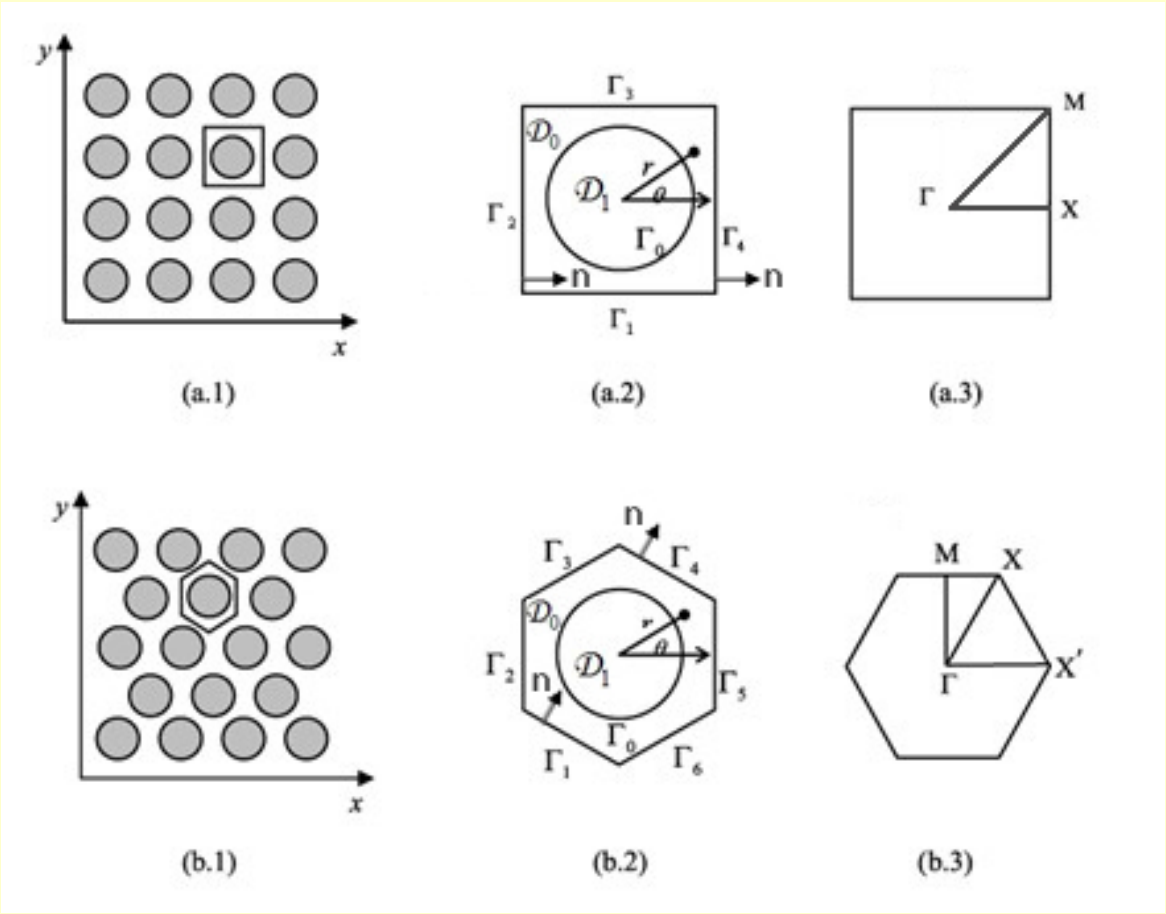
缺点:

- 只适用于圆柱和球形散射体(?)
- 只适用于各向同性介质(?)
- 不适用于表面波(?)

(3) 柱/球波函数展开法-DtN

Dirichlet-to-Neumann (DtN) 映射方法

DtN映射：某特征量与其导数之间的映射关系



DtN映射

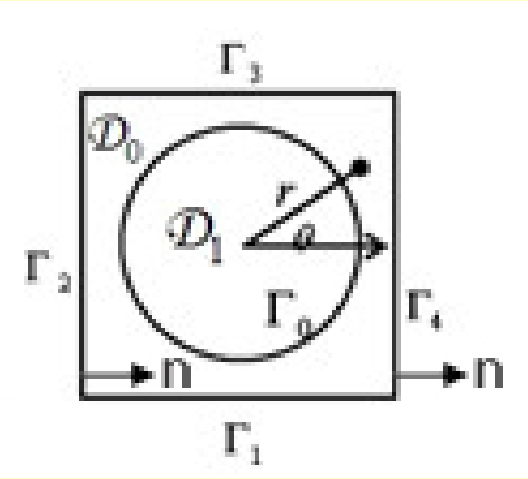
$$\Lambda \cdot \mathbf{u}\big|_{\Gamma} = \partial_{\mathbf{n}} \mathbf{u}\big|_{\Gamma}$$

边界位移　　边界位移的法向导数

(3) 柱/球波函数展开法-DtN

SH波、四方晶格为例：

$$\mu_j \nabla^2 u_{zj}(\mathbf{r}) + \rho_j \omega^2 u_{zj}(\mathbf{r}) = 0, \quad \mathbf{r} \in D_j, \quad j = 0,1$$



柱波函数展开：

$$u(x,y) = \sum_{m=-\infty}^{\infty} C_m \Phi_m(r,\theta), \quad \Phi_m(r,\theta) = \phi_m(r) e^{im\theta}$$

$$\phi_m(r) = \begin{cases} A_m J_m(k_1 r), & r < r_c \\ B_m J_m(k_0 r) + Y_m(k_0 r), & r > r_c \end{cases}$$

界面条件：

$$u_{z1}(\mathbf{r}) = u_{z0}(\mathbf{r}), \qquad \mu_1 \frac{\partial u_{z1}(\mathbf{r})}{\partial \mathbf{n}} = \mu_0 \frac{\partial u_{z0}(\mathbf{r})}{\partial \mathbf{n}}, \qquad \mathbf{r} \in \Gamma_0$$

$\Rightarrow A_m, B_m$

(3) 柱/球波函数展开法-DtN

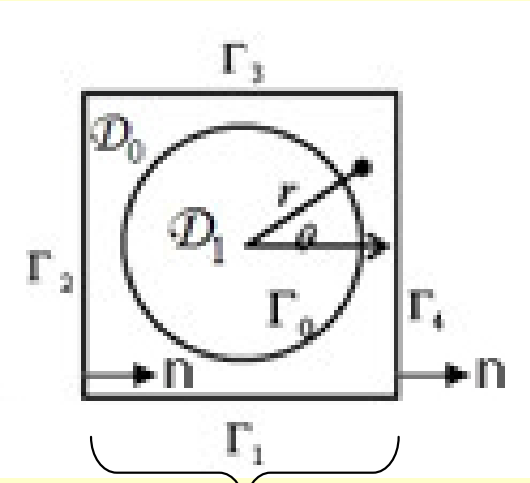
DtN映射：

$$\Lambda u\big|_{\Gamma_k} = \frac{\partial u}{\partial \mathbf{n}}\bigg|_{\Gamma_k}$$

单胞边界配置点：(r_l, θ_l) $l = 0 \sim 4N$

$$\Lambda = \Lambda_2 \Lambda_1^{-1} \qquad (\Lambda_1)_{lm} = \Phi_m(r_l, \theta_l)$$

$$(\Lambda_2)_{lm} = \partial \Phi_m(r_l, \theta_l)/\partial \mathbf{n}(l)$$



N个边界配置点

对应边界上应用**Bloch**定理：

$$u\big|_{\Gamma_3} = \alpha u\big|_{\Gamma_1}, \quad u\big|_{\Gamma_4} = \beta u\big|_{\Gamma_2}, \quad \frac{\partial u}{\partial y}\bigg|_{\Gamma_3} = \alpha \frac{\partial u}{\partial y}\bigg|_{\Gamma_1}, \quad \frac{\partial u}{\partial x}\bigg|_{\Gamma_4} = \beta \frac{\partial u}{\partial x}\bigg|_{\Gamma_2}$$

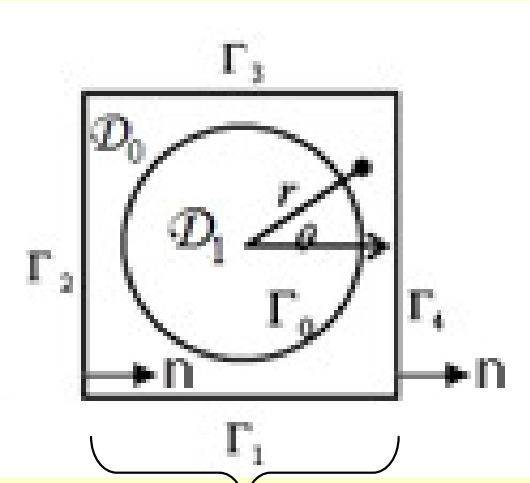
$$\alpha = e^{ik_x a/2} \qquad \beta = e^{ik_y \sqrt{3} a/2}$$

(3) 柱/球波函数展开法-DtN

特征值方程：

$$\left(\lambda^2\mathbf{A}_2+\lambda\mathbf{A}_1+\mathbf{A}_0\right)\mathbf{U}=0$$

$$\mathbf{U}=(u_{\Gamma_1},u_{\Gamma_2})^{\mathrm{T}}$$

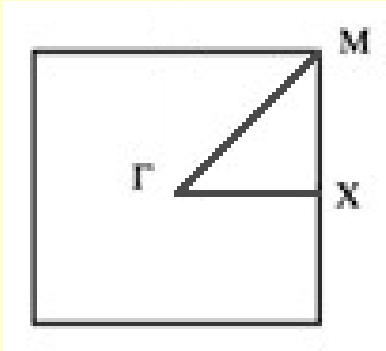


N个边界配置点

BZ区边界上特征值方程线性化：

$$\lambda\begin{bmatrix}\mathbf{A} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{V}\\ \mathbf{U}\end{bmatrix}+\begin{bmatrix}\mathbf{B} & \mathbf{C}\\ \mathbf{-I} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{V}\\ \mathbf{U}\end{bmatrix}=0$$

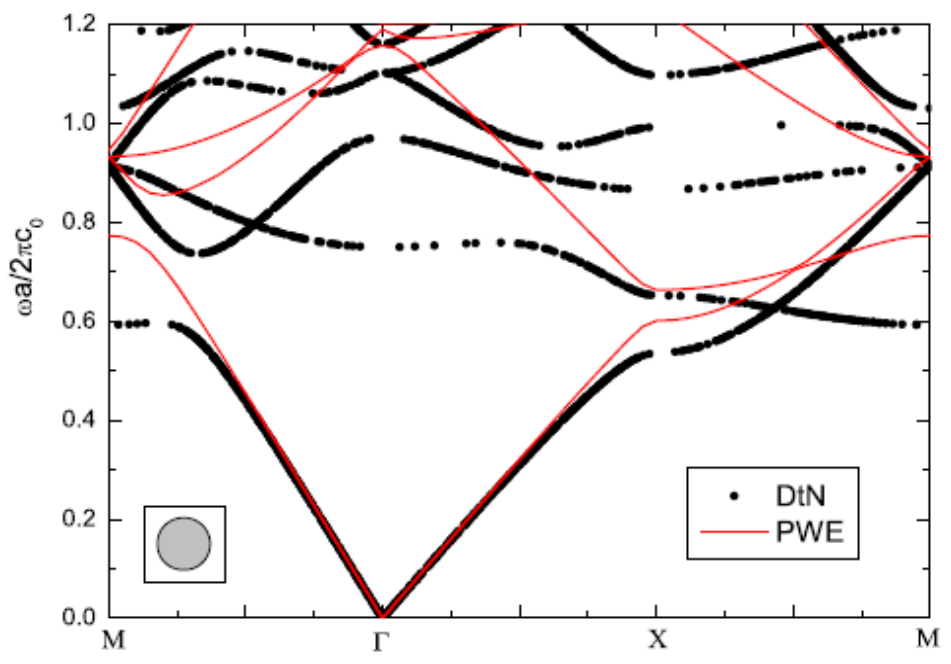
$$\mathbf{V}=\lambda\mathbf{U}$$

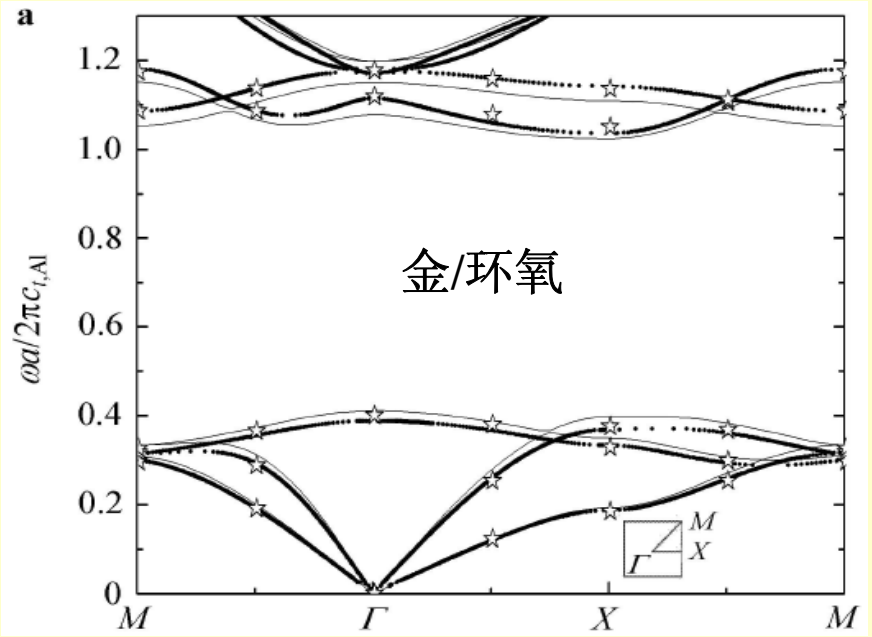


$$|\lambda|=1 \rightarrow \big||\lambda|-1\big|\le\varepsilon \qquad \varepsilon=10^{-6}\sim10^{-8}$$

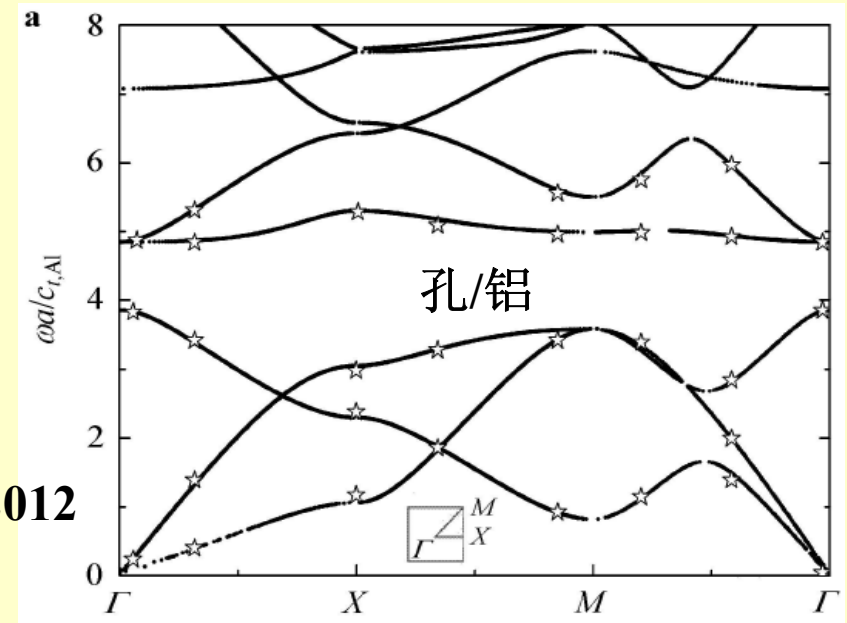
(3) 柱/球波函数展开法-DtN

Li et al. Phys. Scr., 2011
(铝/汞)





Zhen et al. AMS, 2012



(3) 柱/球波函数展开法-DtN

优点:

- 可以计算能带、响应，计算速度快
- 适用于流固混合系统
- 可计算任意频率区间的能带
- 可考虑界面连接的差异，易推广到粘弹性

缺点:

- 只适用于圆柱和球形散射体(?)
- 只适用于各向同性介质(?)
- 不适用于表面波(?)
- 对3维系统不易实施

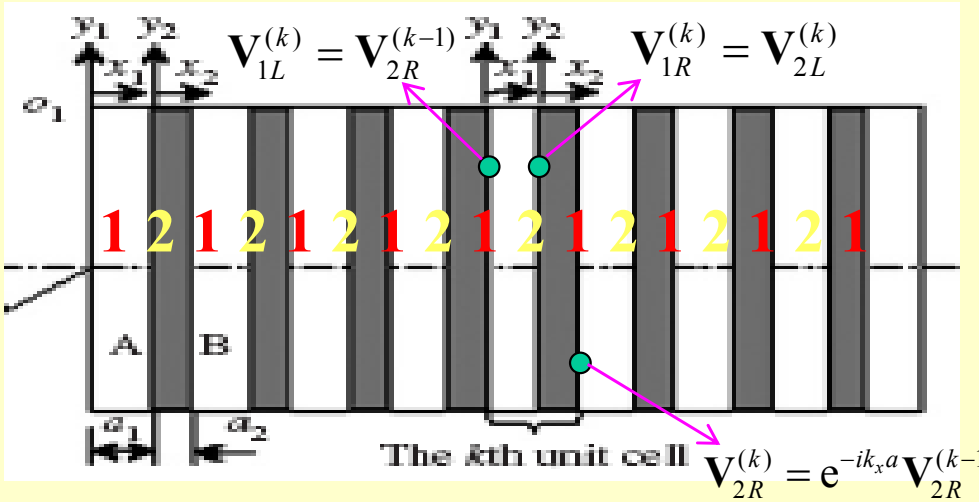
(4) 传递矩阵法(TMM)

主要针对1维系统，界面状态向量之间的传递

第*k*个单胞:

$$\mathbf{V}_{1R}^{(k)} = \mathbf{T}_1'\mathbf{V}_{1L}^{(k)} \qquad \mathbf{V}_{2R}^{(k)} = \mathbf{T}_2'\mathbf{V}_{2L}^{(k)}$$

$$\mathbf{V}_{2R}^{(k)} = \mathbf{T}_k\mathbf{V}_{1L}^{(k)} \qquad (\mathbf{T}_k = \mathbf{T}_2'\mathbf{T}_1')$$



$$\mathbf{V}_{2R}^{(k)} = \mathbf{T}_k\mathbf{V}_{2R}^{(k-1)} \quad (\mathbf{T}_k \text{ is the same for periodic systems})$$

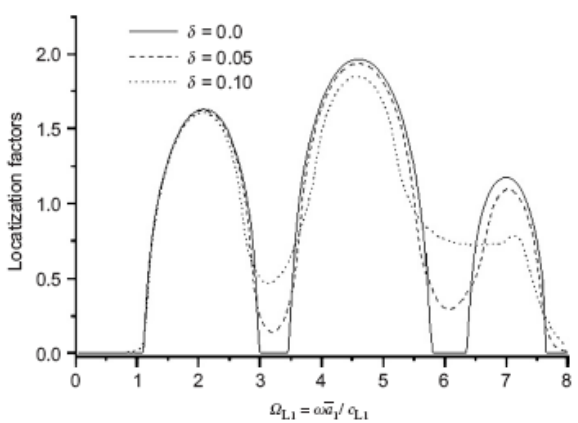
$$\mathbf{V}_{2R}^{(k)} = e^{-ik_x a}\mathbf{V}_{2R}^{(k-1)} \Longrightarrow \boxed{\left|\mathbf{T} - e^{-ik_x a}\mathbf{I}\right| = 0} \quad \text{(eigenvalue eq.)}$$

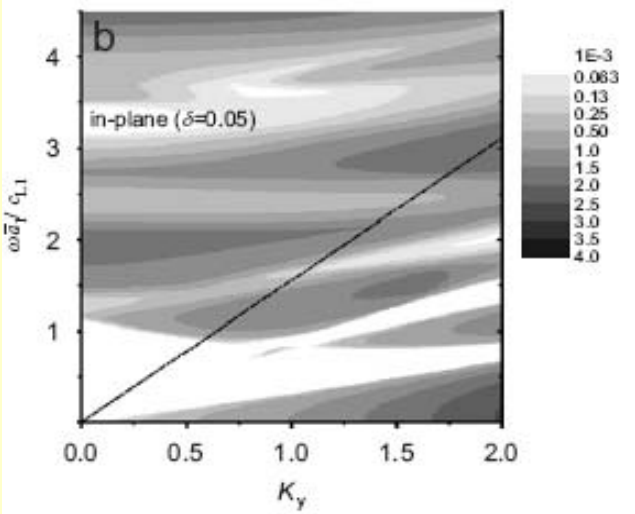
Response: $\mathbf{V}_n = \mathbf{T}_{total}\mathbf{V}_0 \quad (\mathbf{T}_{total} = \mathbf{T}_n\mathbf{T}_{n-1}\cdots\mathbf{T}_k\cdots\mathbf{T}_1 = \mathbf{T}^n)$

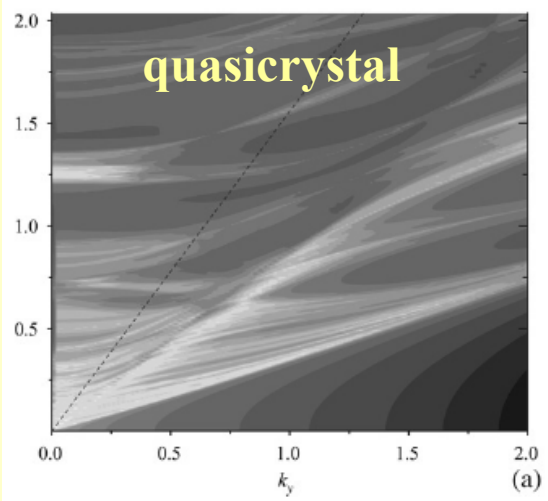
(4) 传递矩阵法(TMM)

优点:

- 可计算能带/传输谱/局部化因子
- 适用于周期/非周期
- 适用于各向异性、不同界面连接
- 适用于流-固混合体系







Localization factor for randomly disordered system

Chen, Wang, et al. Phy. B, 2007; SSC, 2007 (Pb/Epoxy)

(4) 传递矩阵法(TMM)

缺点:

- 只适用于1维系统
- 难适用于表面波
- 高频响应计算不稳定

提高计算稳定性的改进方法:

Delta Matrix Method

Scattering Matrix Method

Global Matrix Method

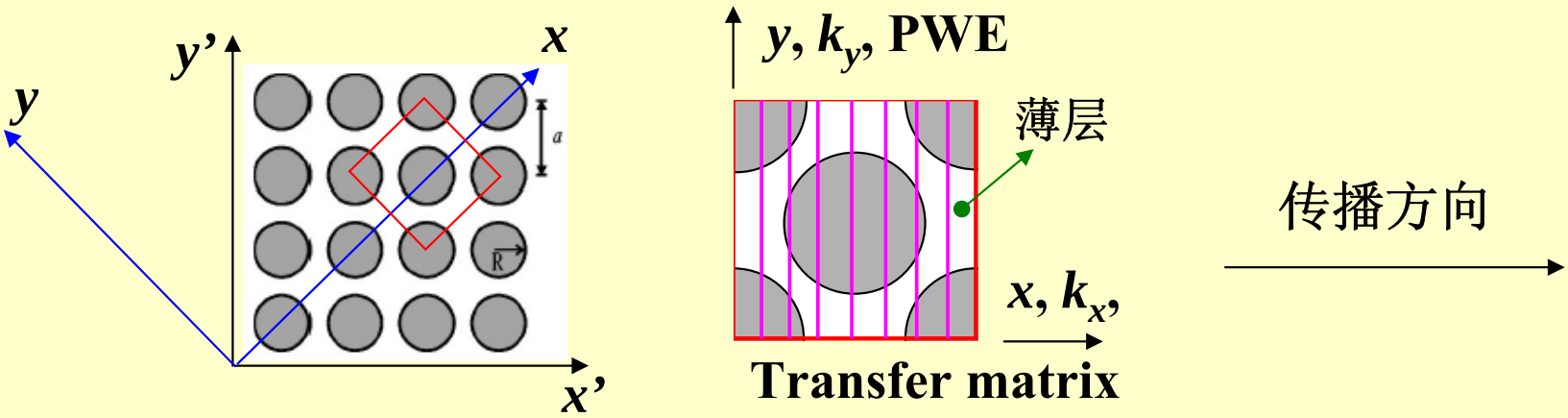
Stiffness Matrix Method

(4) 传递矩阵法(TMM)

推广用于计算2维和3维系统的响应

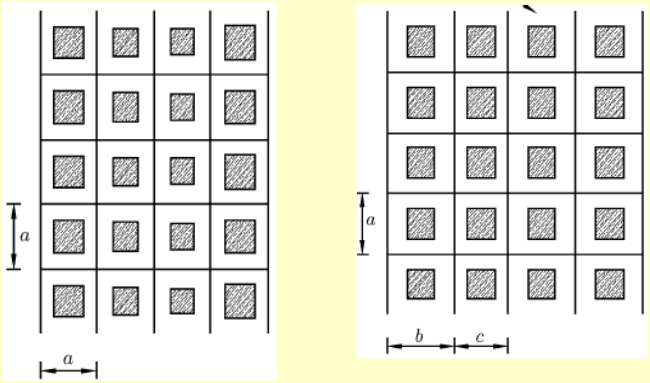
—基于平面波展开的传递矩阵法:

$$\mathbf{u}(x,y)=\mathrm{e}^{ik_y y}\sum_G \mathbf{u}_{k_y}(G)\mathrm{e}^{iGy}\mathrm{e}^{ik_x x}$$

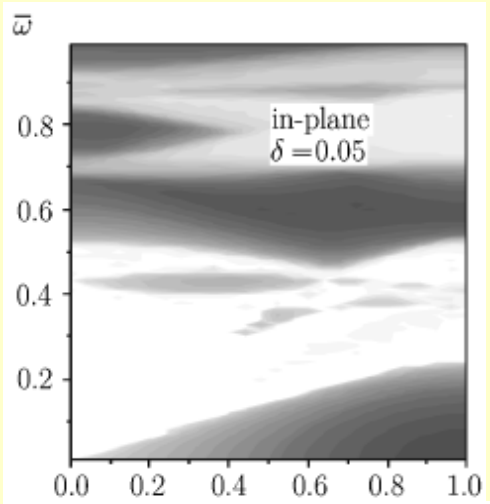


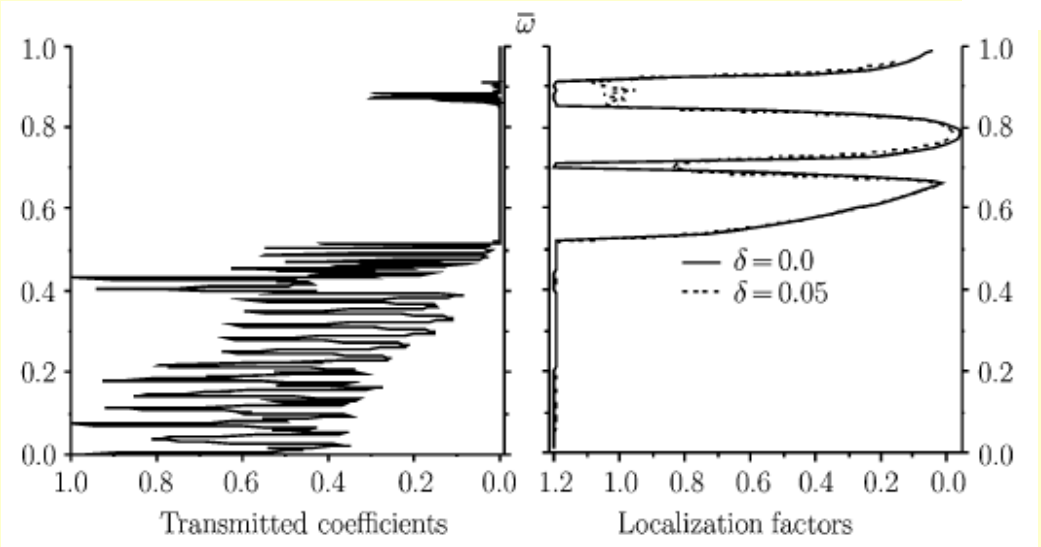
(4) 传递矩阵法(TMM)

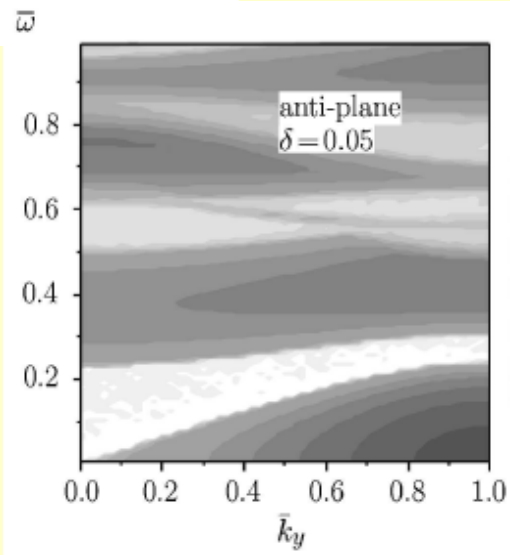
利用基于平面波展开的传递矩阵法计算单向失谐的2维系统



Chen, Wang, et al, AMSS, 2008







(5) 有限差分法(FDM)

— 时域有限差分法(FDTD)

抛物型方程组:

$$\begin{cases} \rho(\mathbf{r})\ddot{\mathbf{u}}(\mathbf{r},t) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{r},t) \\ \boldsymbol{\sigma}(\mathbf{r},t) = \mathbb{C}:\nabla\mathbf{u}(\mathbf{r},t) \end{cases} \quad (*)$$

(Tanaka, et al. PRB, 2000
TT Wu, et al. IEEE, 2006)

双曲型方程组:

$$\begin{cases} \rho(\mathbf{r})\dot{\mathbf{v}}(\mathbf{r},t) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{r},t) \\ \dot{\boldsymbol{\sigma}}(\mathbf{r},t) = \mathbb{C}:\nabla\mathbf{v}(\mathbf{r},t) \end{cases}$$

(G Wang, et al. APS, 2003
XX Su, et al. PhysB, 2010)
计算精度较高

$$\left(\mathbf{v} = \dot{\mathbf{u}}\right)$$

(5) 有限差分法(FDM)

Bloch变换/定理：

$$\mathbf{u}(\mathbf{r},t)=\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{U}(\mathbf{r},t)$$
$$\mathbf{v}(\mathbf{r},t)=\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{V}(\mathbf{r},t)$$
$$\boldsymbol{\sigma}(\mathbf{r},t)=\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{S}(\mathbf{r},t)$$

(满足周期条件)

抛物型方程组：

$$\begin{cases}\rho(\mathbf{r})\ddot{\mathbf{U}}(\mathbf{r},t)=(\nabla+i\mathbf{k})\cdot\mathbf{S}(\mathbf{r},t)\\ \mathbf{S}(\mathbf{r},t)=\mathbb{C}:(\nabla+i\mathbf{k})\otimes\mathbf{U}(\mathbf{r},t)\end{cases}$$

(**)

双曲型方程组：

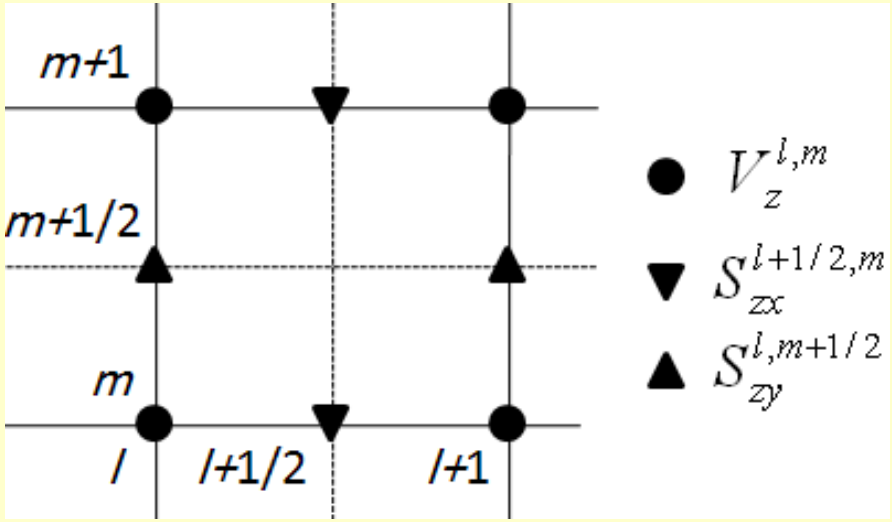
$$\begin{cases}\rho(\mathbf{r})\dot{\mathbf{V}}(\mathbf{r},t)=(\nabla+i\mathbf{k})\cdot\mathbf{S}(\mathbf{r},t)\\ \dot{\mathbf{S}}(\mathbf{r},t)=\mathbb{C}:(\nabla+i\mathbf{k})\otimes\mathbf{V}(\mathbf{r},t)\end{cases}$$

(5) 有限差分法(FDM)

中心差分:

$$\frac{df(x)}{dx}=\frac{f(x+\Delta x/2)-f(x-\Delta x/2)}{\Delta x}+O\left[(\Delta x)^2\right]$$

交替采样:



(5) 有限差分法(FDM)

时间递推/迭代:

满足Courant稳定性条件:

$$\Delta t \le \frac{1}{c\sqrt{(\Delta x)^{-2}+(\Delta y)^{-2}+(\Delta z)^{-2}}}$$

(**c**: 非均匀介质中的最大波速)

避免数值色散: $\Delta t \le T/12$

$$\Delta x, \Delta y, \Delta z \le \lambda/12$$

(**T**, λ: 波的周期和波长)

(5) 有限差分法(FDM)

初始条件:

点脉冲源或分布脉冲源，能够激发所有模态的波。

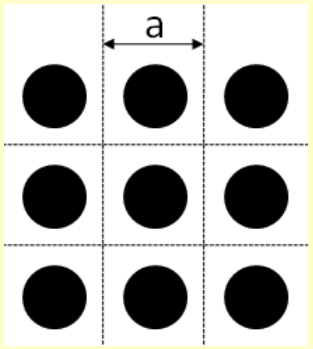
(*) ：初始激励满足Bloch条件；

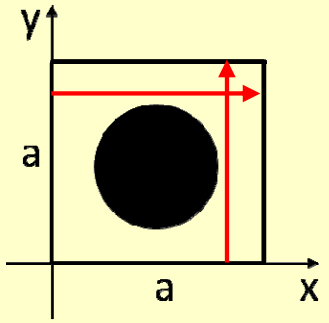
(**)：初始激励满足周期条件。

(5) 有限差分法(FDM)

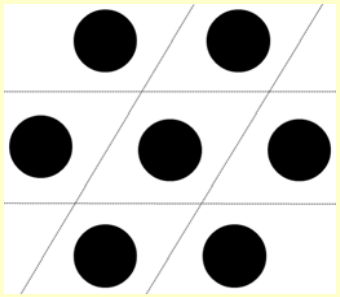
周期性边界条件:

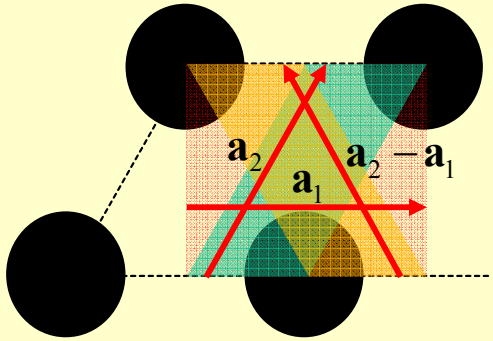
(*) ： 每时间步满足Bloch条件





(**) ： 每时间步满足周期条件



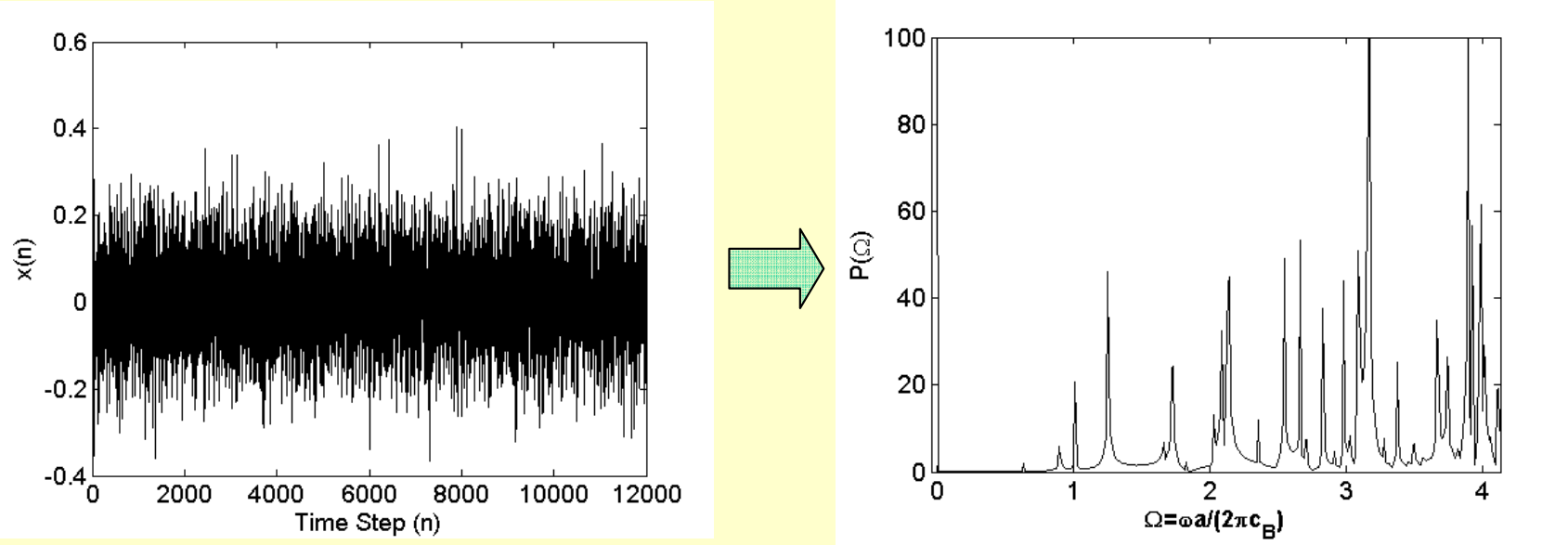


(5) 有限差分法(FDM)

数据后处理(获取能带):

FFT

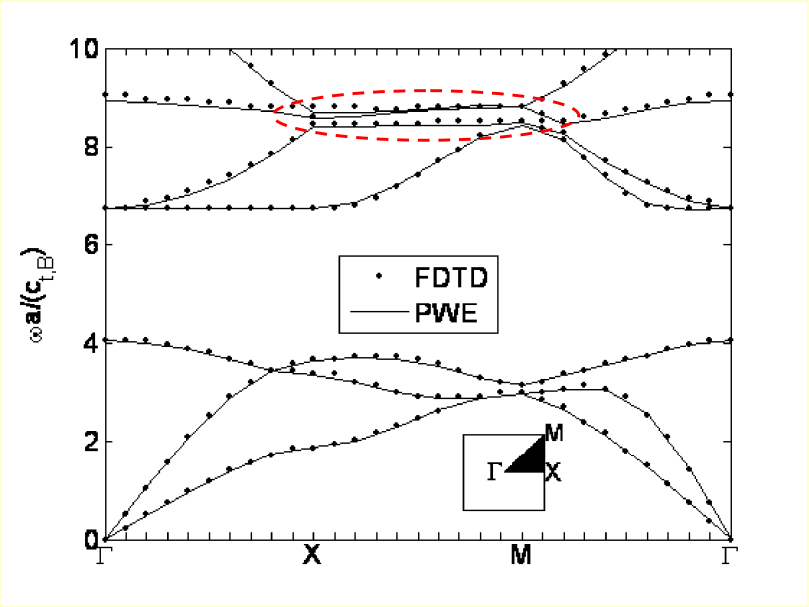
时间序列 ⟶ 频谱

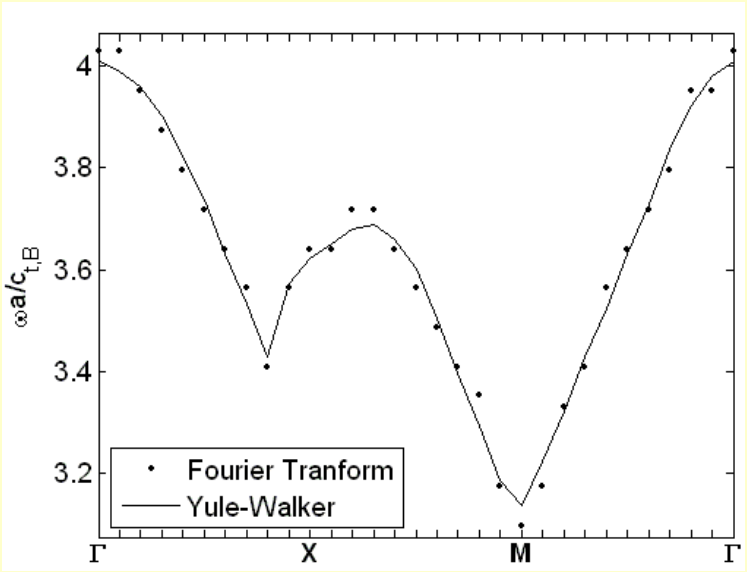


(5) 有限差分法(FDM)

提高效率的某些后处理方法:

高分辨率谱估计方法:　　精确估算特征频率

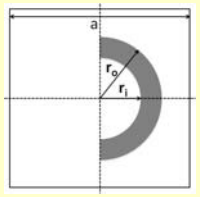




钢/环氧树脂　　Su, Wang, et al. 人工晶体, 2009

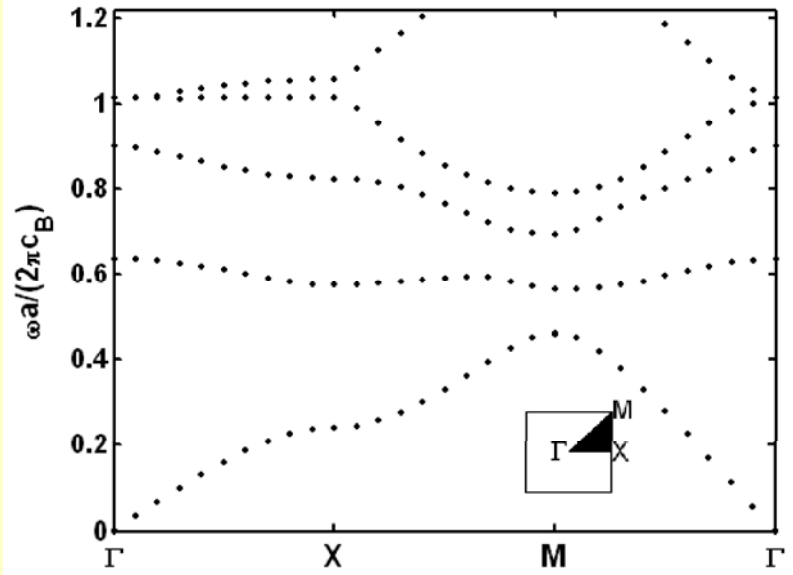
(5) 有限差分法(FDM)

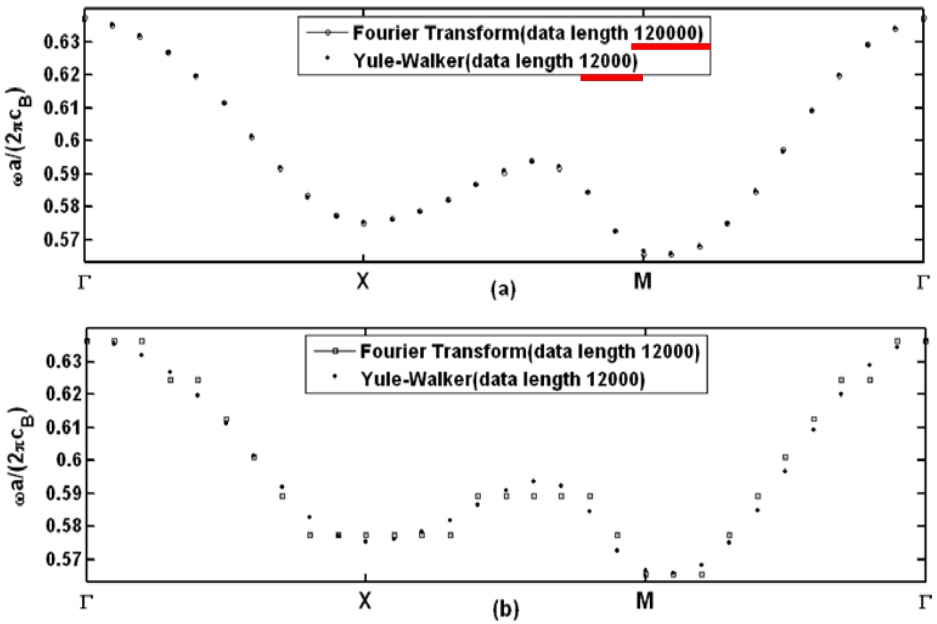
高分辨率谱估计方法：　明显减少FDTD的迭代步数



刚体/空气

TJ Lu, et al. Sci C, 2009

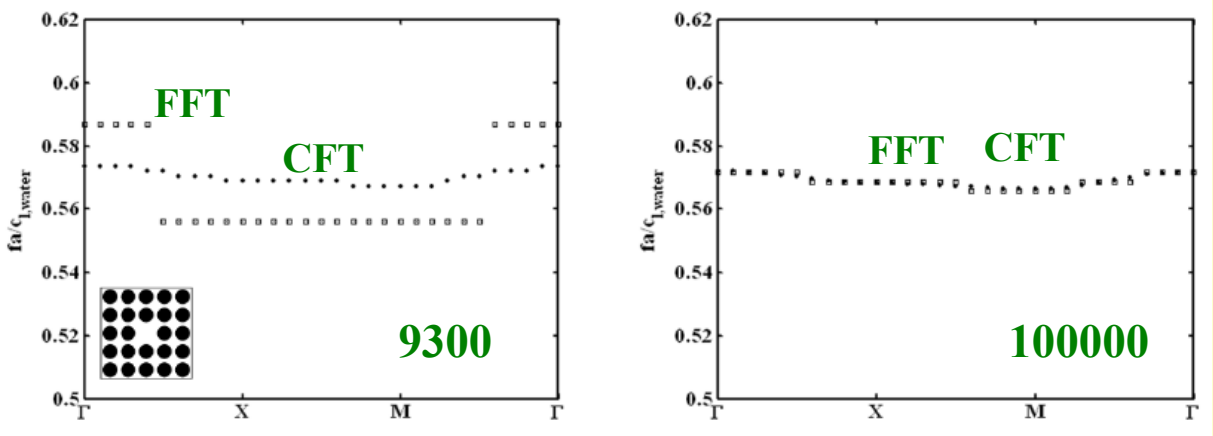




Su, Wang, et al. PhysB, 2010

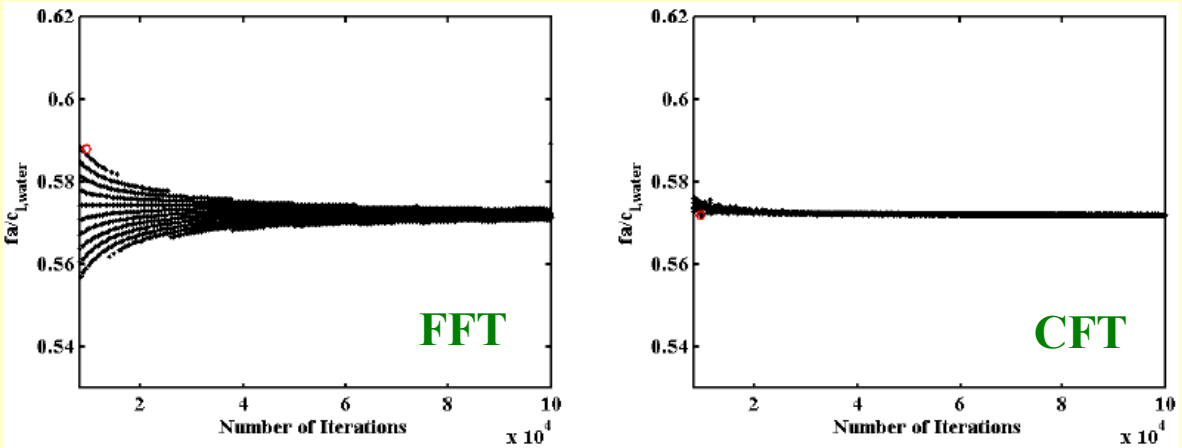
(5) 有限差分法(FDM)

频率细化技术 (CFT)： 计算缺陷态明显减少FDTD的迭代步数



钢/水

Su, Wang. PhysB, 2010



(5) 有限差分法(FDM)

特点:

1. 简单易行
2. 适用性广泛（3D、流/固、散射体形状、各向异性）
3. 易于实现并行
4. 需要后处理，某些情况要谨慎
5. 表面波、Lamb波计算较困难
6. 流体夹杂的情况计算慢、结果不理想
7. 界面连接的差异?

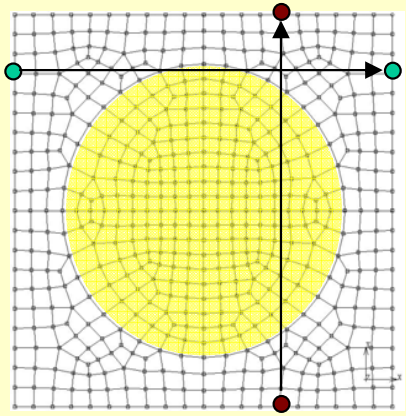
(6) 有限元方法(FEM)

方法一：

波动方程:

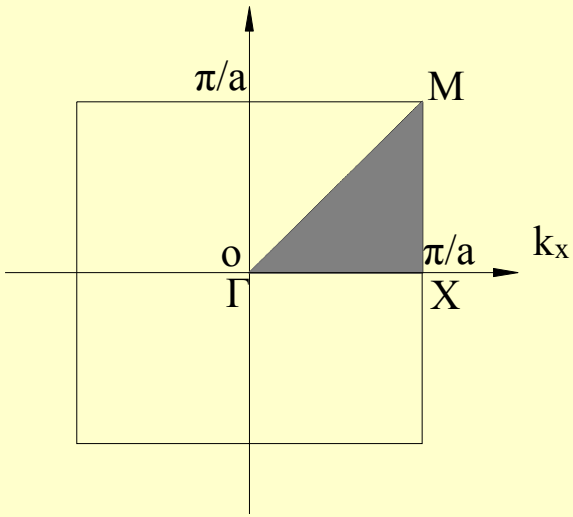
$$\nabla \cdot (\mathbb{C}(\mathbf{r}) : \nabla \mathbf{u}(\mathbf{r})) + \rho(\mathbf{r})\omega^2 \mathbf{u}(\mathbf{r}) = 0$$

Bloch定理: $\mathbf{u}(\mathbf{r}) = e^{i(\mathbf{k}\cdot\mathbf{r})}\mathbf{u}_{\mathbf{k}}(\mathbf{r})$



单胞离散:

$(\mathbf{K}-\omega^2\mathbf{M})\mathbf{U}=0$



边界上对应点施加**Bloch**条件:



(6) 有限元方法(FEM)

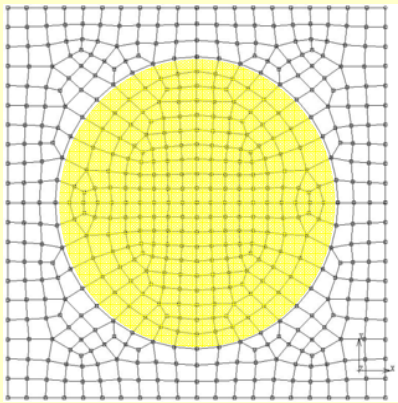
求解特征值方程:

1、利用商业软件Comsol：支持复数运算，直接求解

2、利用商业软件Abaqus：不支持复数运算，
实部虚部分开求解，划分重网格

$$\left(\begin{bmatrix}\mathbf{K}_R & -\mathbf{K}_I \\ \mathbf{K}_I & \mathbf{K}_R\end{bmatrix} - \omega^2 \begin{bmatrix}\mathbf{M}_R & -\mathbf{M}_I \\ \mathbf{M}_I & \mathbf{M}_R\end{bmatrix}\right)\begin{bmatrix}\mathbf{u}_R \\ \mathbf{u}_I\end{bmatrix} = 0$$

$$\begin{bmatrix}\mathbf{u}_R(\mathbf{r}) \\ \mathbf{u}_I(\mathbf{r})\end{bmatrix} = \begin{bmatrix}\cos(\mathbf{k}\cdot\mathbf{a}) & \sin(\mathbf{k}\cdot\mathbf{a}) \\ -\sin(\mathbf{k}\cdot\mathbf{a}) & \cos(\mathbf{k}\cdot\mathbf{a})\end{bmatrix}\begin{bmatrix}\mathbf{u}_R(\mathbf{r}+\mathbf{a}) \\ \mathbf{u}_I(\mathbf{r}+\mathbf{a})\end{bmatrix}$$



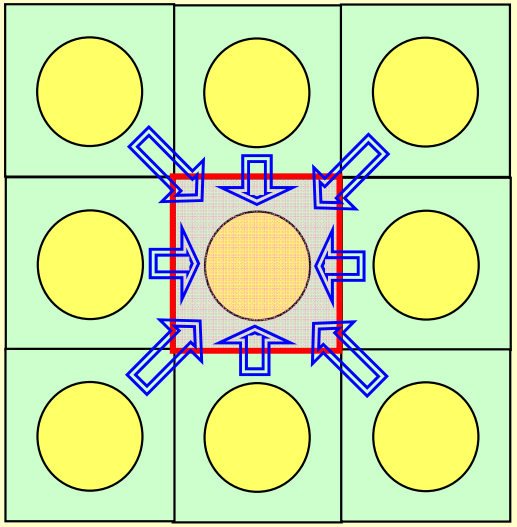
(6) 有限元方法(FEM)

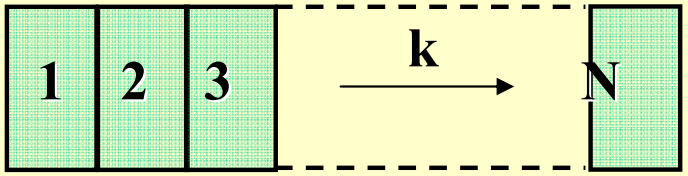
证明上述实施过程能够保证整个结构上每一个节点的场量均满足**Bloch**定理:

$$(\mathbf{K}-\omega^2\mathbf{M})\mathbf{U}=0 \quad \text{(整个无限周期结构离散)}$$

$$\mathbf{U}=\left[\mathbf{u}^{(1)},\mathbf{u}^{(2)},\cdots,\mathbf{u}^{(j)},\cdots,\mathbf{u}^{(N)}\right]^T$$

$$\mathbf{K}=\begin{bmatrix}\mathbf{K}_{11} & \mathbf{K}_{12} & \cdots & \mathbf{K}_{1N}\\ \mathbf{K}_{21} & \mathbf{K}_{22} & \cdots & \mathbf{K}_{2N}\\ \cdots & \cdots & & \\ \mathbf{K}_{N1} & \mathbf{K}_{N2} & \cdots & \mathbf{K}_{NN}\end{bmatrix} \quad \mathbf{M}=\begin{bmatrix}\mathbf{M}_{11} & \mathbf{M}_{12} & \cdots & \mathbf{M}_{1N}\\ \mathbf{M}_{21} & \mathbf{M}_{22} & \cdots & \mathbf{M}_{2N}\\ \cdots & \cdots & \cdots & \cdots\\ \mathbf{M}_{N1} & \mathbf{M}_{N2} & \cdots & \mathbf{M}_{NN}\end{bmatrix}$$





$$\mathbf{u}^{(j-1)}=e^{-i(\mathbf{k}\cdot\mathbf{r})}\mathbf{u}^{(j)} \quad ?$$

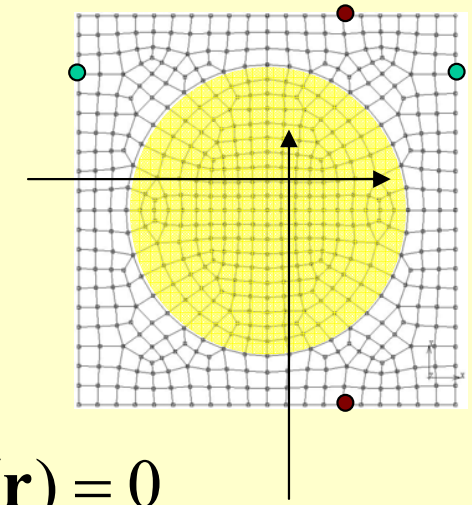
证明详见**Li, et al, J. Compu. Acoust., 2012,**
DOI No: 10.1142/S0218396X12500142

(6) 有限元方法(FEM)

方法二：

波动方程：$\nabla\cdot(\mathbb{C}(\mathbf{r}):\nabla\mathbf{u}(\mathbf{r}))+\rho(\mathbf{r})\omega^2\mathbf{u}(\mathbf{r})=0$

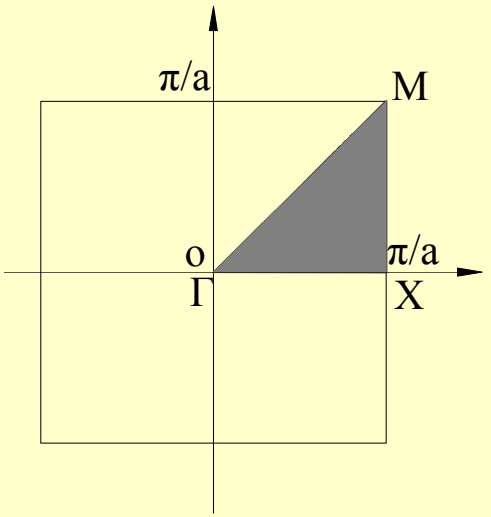
Bloch定理： $\mathbf{u}(\mathbf{r})=e^{i(\mathbf{k}\cdot\mathbf{r})}\mathbf{u}_\mathbf{k}(\mathbf{r})$



$$(\nabla+i\mathbf{k})\cdot[\mathbb{C}(\mathbf{r}):(\nabla+i\mathbf{k})\otimes\mathbf{u}_\mathbf{k}(\mathbf{r})]+\rho(\mathbf{r})\omega^2\mathbf{u}_\mathbf{k}(\mathbf{r})=0$$

单胞离散：$[\mathbf{K}(k_x^2+k_y^2,k_x,k_y)-\omega^2\mathbf{M}]\mathbf{U}_\mathbf{k}=0$

边界上对应点施加周期：$\mathbf{U}_\mathbf{k}(\mathbf{r})=\mathbf{U}_\mathbf{k}(\mathbf{r}+\mathbf{a})$



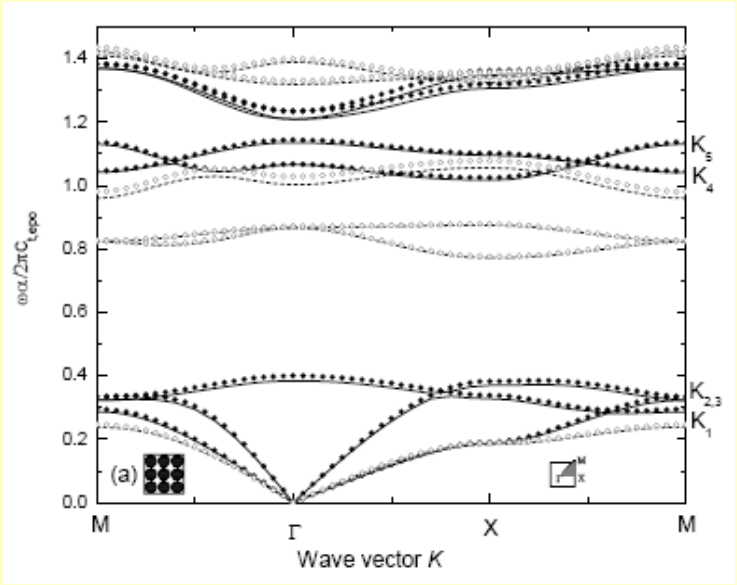
可利用Comsol的偏微分方程模块求解。

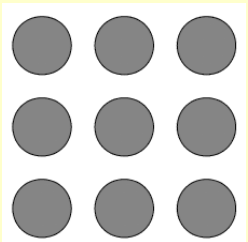
(6) 有限元方法(FEM)

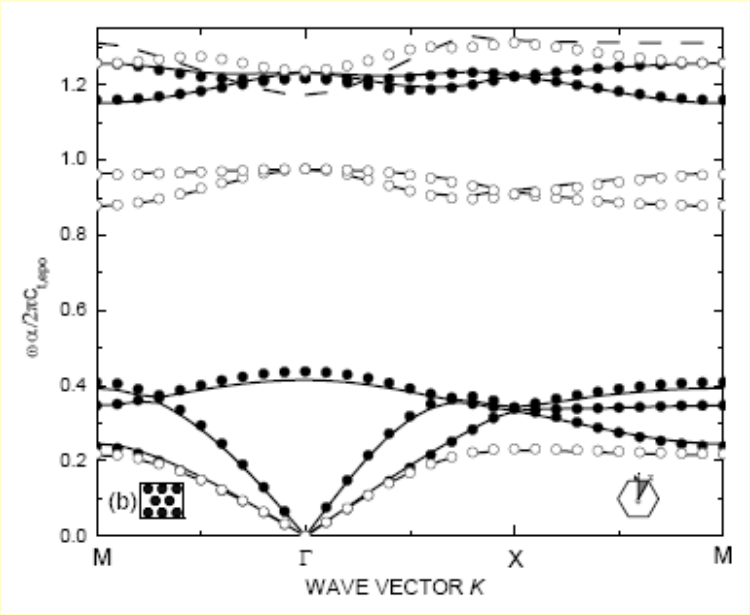
特点：

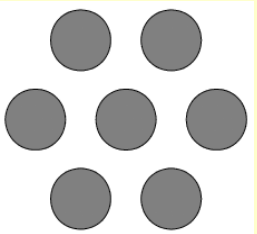
- 结果精度高

实线: **FEM (1058个CPE4单元)**
散点: **PWE (1089个平面波)**







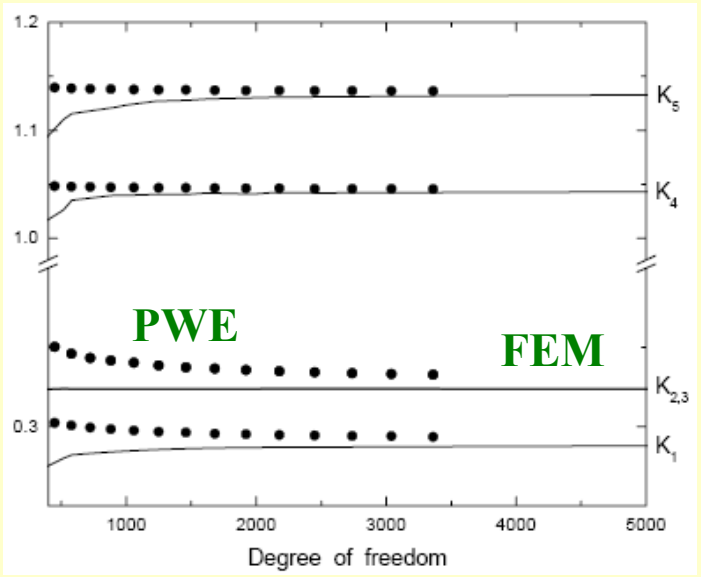


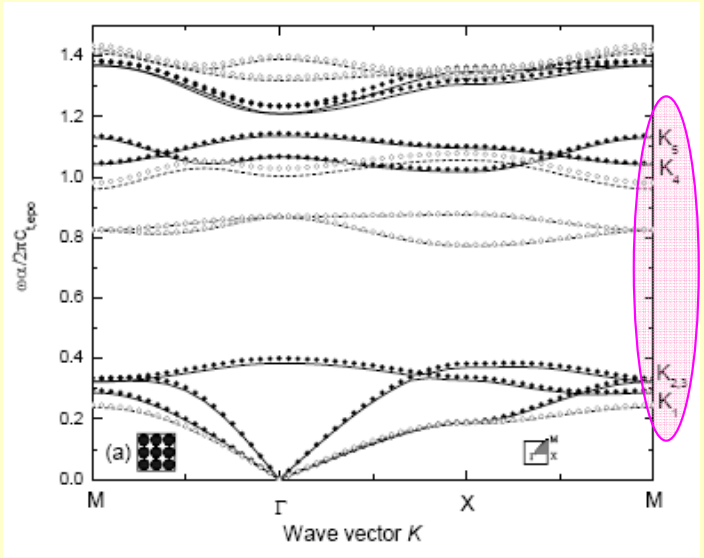
金/环氧 (f=0.44)

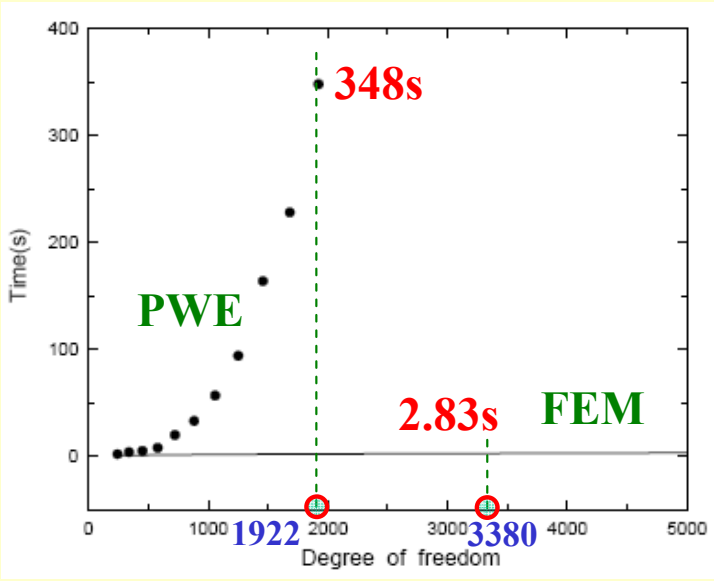
(6) 有限元方法(FEM)

- 收敛性好、计算速度快

(PC/2.13GHz/8G)



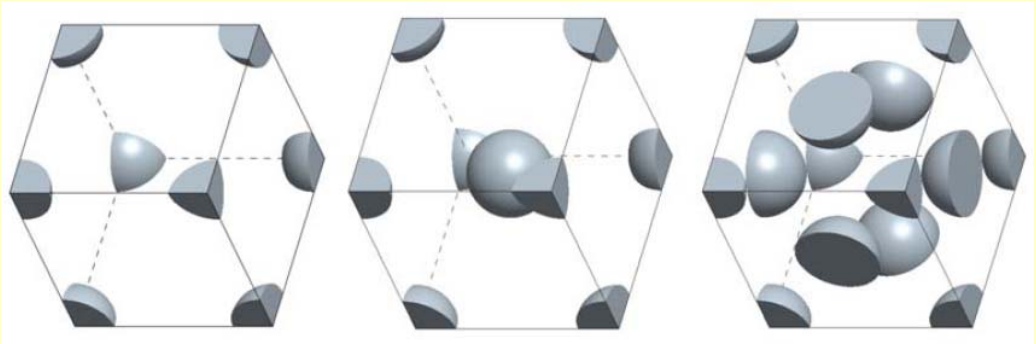


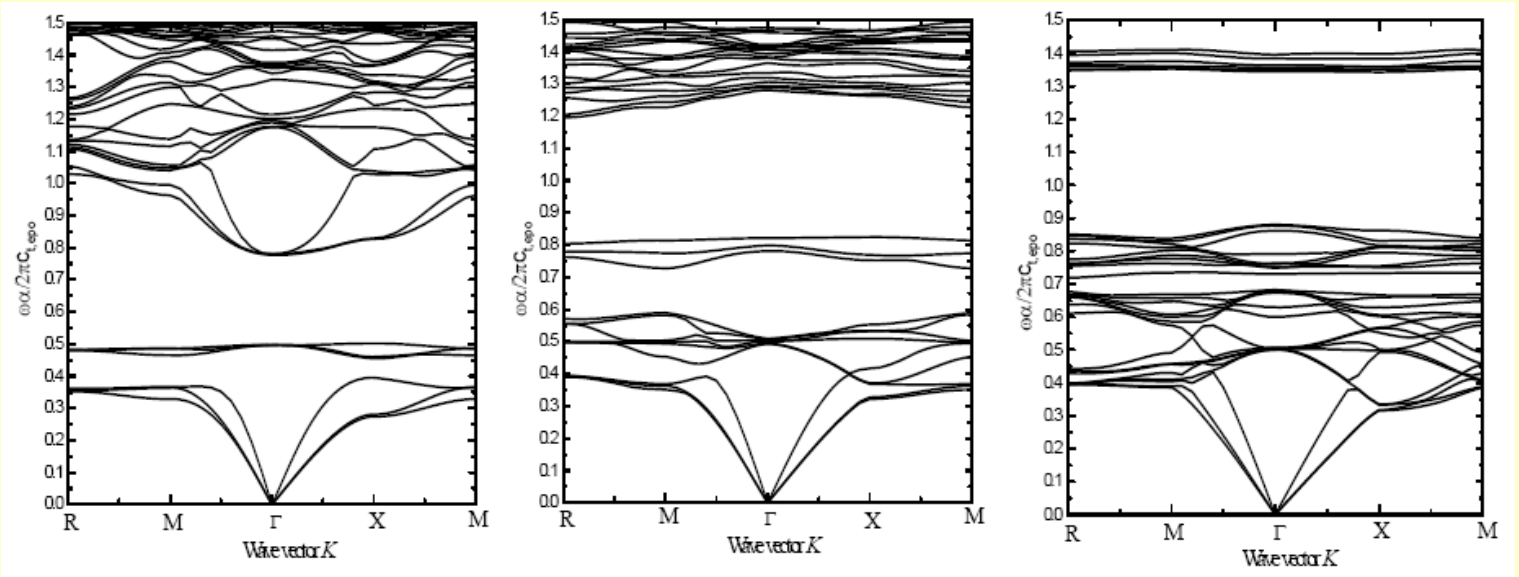


(6) 有限元方法(FEM)

- 适用于三维体系

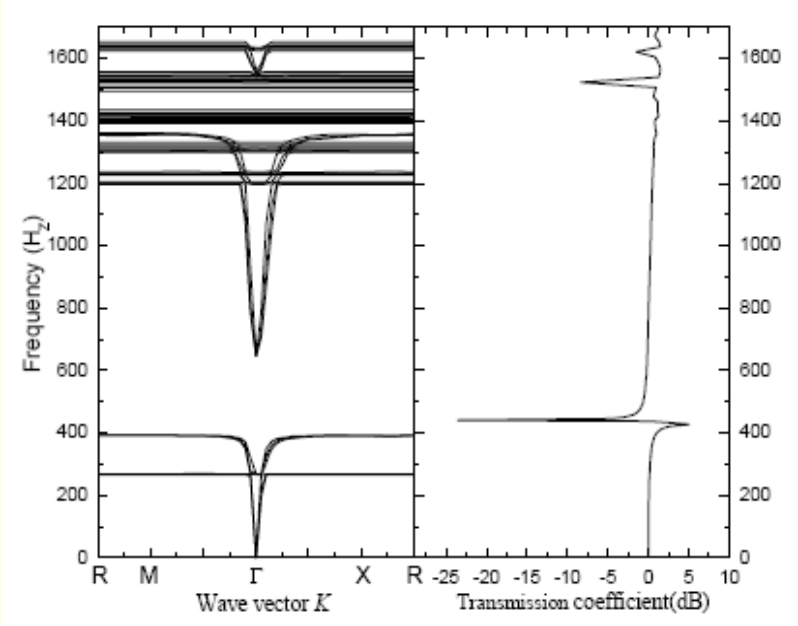
sc bcc fcc

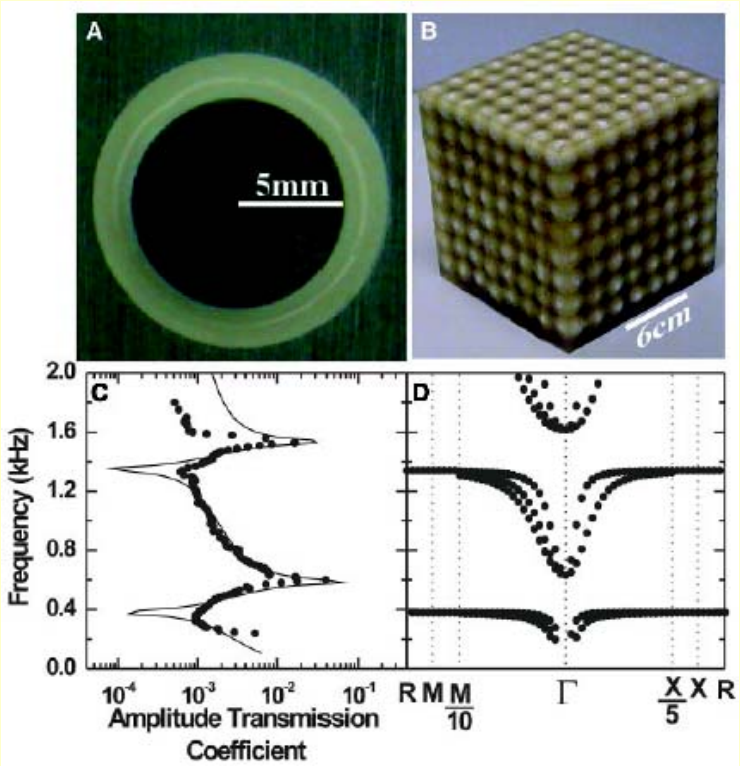




(6) 有限元方法(FEM)

- 适用于三相体系



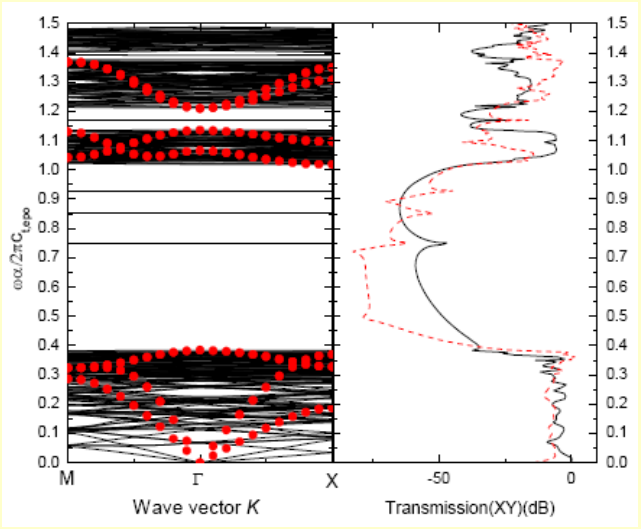


(Liu, et.al. Science, 2000)

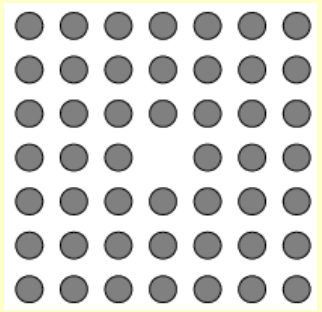
橡胶涂层铅球/环氧

(6) 有限元方法(FEM)

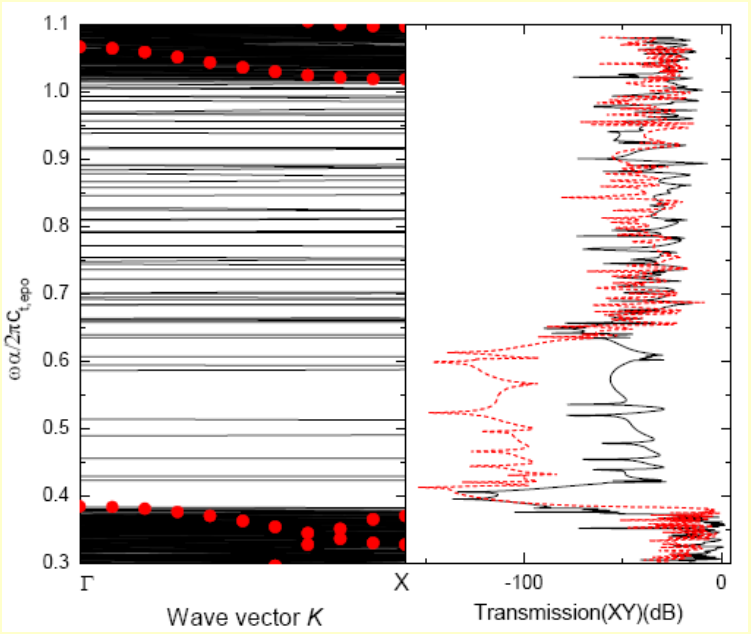
- 适用于缺陷体系

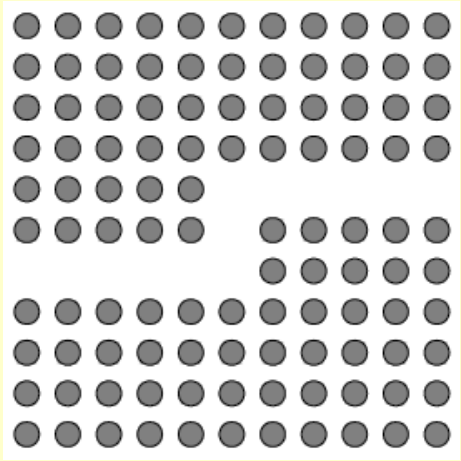


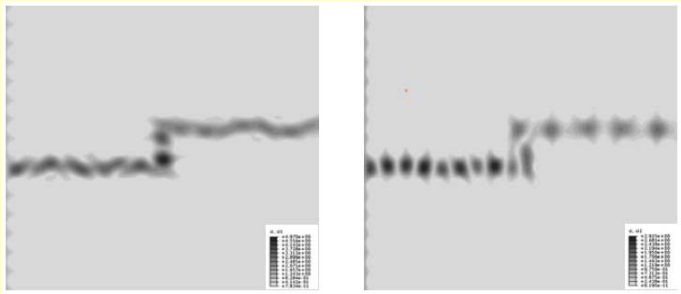
点缺陷



金/环氧 (f=0.44)







更复杂的
Z字型缺陷

(6) 有限元方法(FEM)

- 适用于流/固混合体系

$$C_{11}^{-1}(\mathbf{r})\omega^2 p(\mathbf{r}) = \nabla\cdot[\rho^{-1}(\mathbf{r})\nabla p(\mathbf{r})]$$

p：流体压力势

$$\frac{1}{\rho_f}\frac{\partial p}{\partial \mathbf{r}}\cdot\mathbf{n}^- + \ddot{\mathbf{u}}\cdot\mathbf{n}^- = 0$$

n：边界单位法向量

$$\begin{bmatrix}\mathbf{K}_s & \mathbf{Q}^T\\ 0 & \mathbf{K}_f\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix} = \omega^2\begin{bmatrix}\mathbf{M}_s & 0\\ -\mathbf{Q} & \mathbf{M}_f\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix}$$

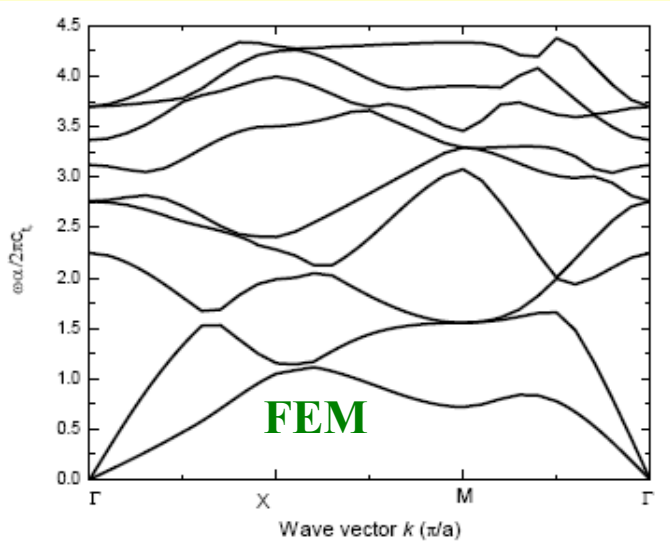
K：刚度矩阵

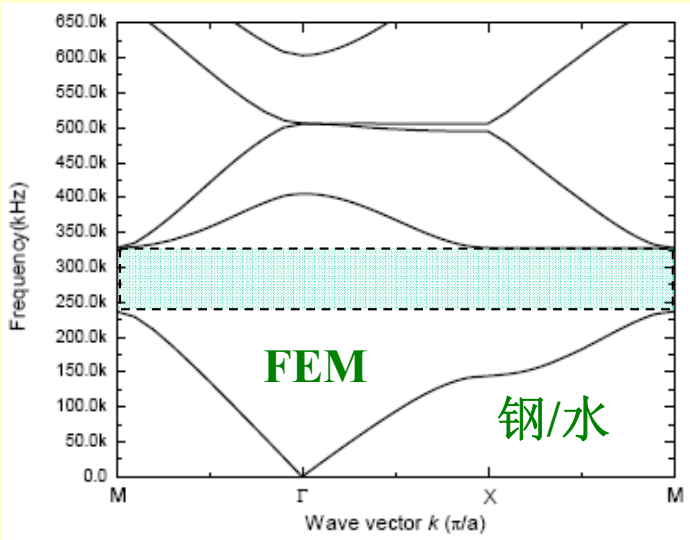
M：质量矩阵

Q：流固耦合矩阵

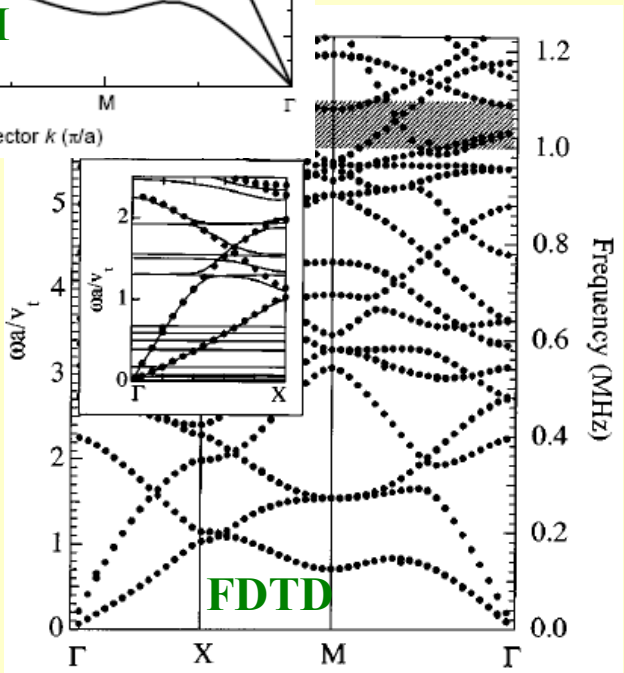
流体单元：AC2D4

(6) 有限元方法(FEM)

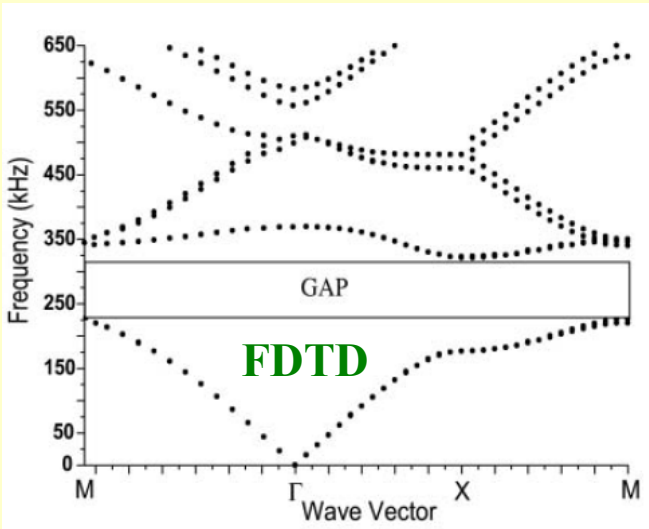




水银/铝



(Tanaka, et al. PRB, 2000)



(Khelif, et al. Z.Krist, 2005)

(6) 有限元方法(FEM)

优点：

1. 简单易行（商业化软件）
2. 适用性广泛（3D、流/固）
3. 能计算较大的体系（缺陷）
4. 结果精确、速度快

待解决的问题：

1. 三维缺陷体系、表面波
2. 界面效应、高频能带结构计算

(7) 边界元方法(BEM)

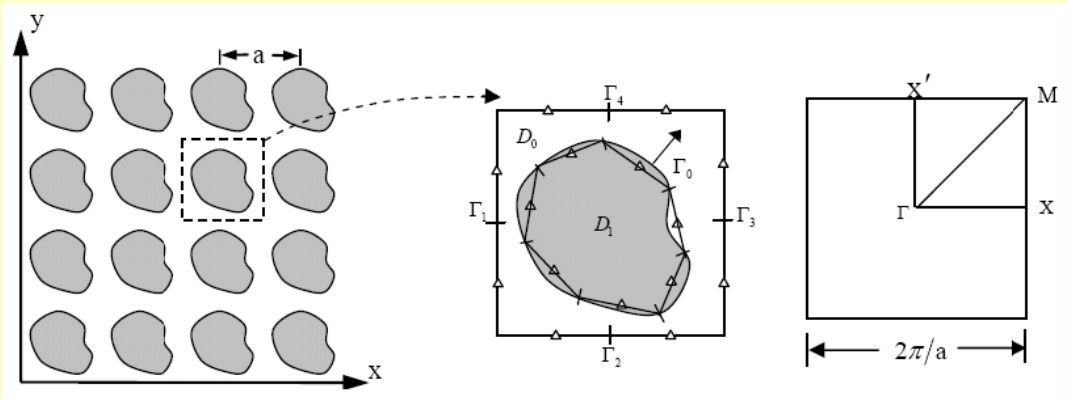
方法一：

弹性动力学基本方程（平面问题）：

$$\lambda\frac{\partial}{\partial x_\alpha}\left(\frac{\partial u_\beta}{\partial x_\beta}\right)+\mu\frac{\partial}{\partial x_\beta}\left[\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}\right]+\rho\omega^2 u_\alpha=0 \qquad \alpha,\beta=x,y$$

Bloch条件： $\mathbf{u}(\mathbf{r}+\mathbf{a})=e^{i\mathbf{k}\cdot\mathbf{a}}\mathbf{u}_\mathbf{k}(\mathbf{r})$

界面连续条件： $\mathbf{u}_1(\mathbf{r})=\mathbf{u}_0(\mathbf{r}),\quad \mathbf{T}_1(\mathbf{r})=\mathbf{T}_0(\mathbf{r}),\quad \mathbf{r}\in\Gamma_0$



$\left.\begin{matrix}\mathbf{T}_1(\mathbf{r})\\ \mathbf{T}_0(\mathbf{r})\end{matrix}\right\}$ are the traction vectors

(7) 边界元方法(BEM)

边界积分方程（**BIE**）：

$$c_{\alpha\beta}u_\beta(\mathbf{x}_Q)+\int_\Gamma s^*_{\alpha\beta}(\mathbf{x}_Q;\mathbf{x}_P)\cdot u_\beta(\mathbf{x}_P)d\Gamma_P=\int_\Gamma v^*_{\alpha\beta}(\mathbf{x}_Q;\mathbf{x}_P)\cdot t_\beta(\mathbf{x}_P)d\Gamma_P \qquad c_{\alpha\beta}=1/2\,\delta_{\alpha\beta}$$

基本解：

$$v^*_{\alpha\beta}(\mathbf{x}_Q;\mathbf{x}_P)=\frac{1}{4\rho\omega^2}\left\{\left[H_0^{(1)}(k_t r)-H_0^{(1)}(k_l r)\right]_{,\alpha\beta}+k_t^2\delta_{\alpha\beta}H_0^{(1)}(k_t r)\right\}$$

$$s^*_{\alpha\beta}(\mathbf{x}_Q;\mathbf{x}_P)=\sigma^*_{\alpha\beta\gamma}(\mathbf{x}_Q;\mathbf{x}_P)\cdot n_\gamma \qquad \sigma^*_{\alpha\beta\gamma}=E_{\alpha\beta\xi\eta}v^*_{\xi\gamma,\eta} \qquad E_{\alpha\beta\xi\eta}=\lambda\delta_{\alpha\beta}\delta_{\xi\eta}+\mu\left(\delta_{\alpha\xi}\delta_{\beta\eta}+\delta_{\alpha\eta}\delta_{\beta\xi}\right)$$

边界离散：

$$\sum_{j=1}^{N}\left[\frac{1}{2}\delta_{\alpha\beta}\delta_{ij}+\int_{\Gamma_j}s^*_{\alpha\beta}(i;j)d\Gamma_j\right](u_\beta)_j-\sum_{j=1}^{N}\left[\int_{\Gamma_j}v^*_{\alpha\beta}(i;j)d\Gamma_j\right](t_\beta)_j=0,\ i=1,2,\cdots,N$$

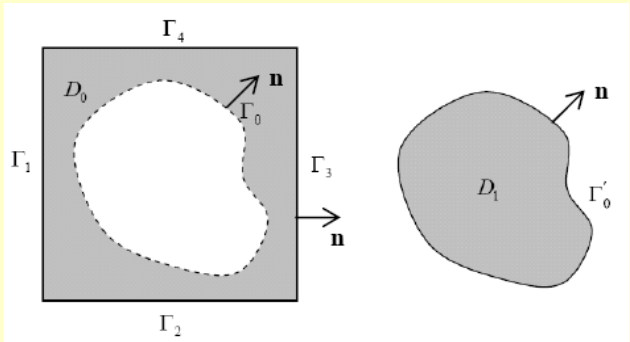
$$\mathbf{HU}+\mathbf{GT}=0 \qquad (\mathbf{U})_j=\left[(u_x)_j,(u_y)_j\right]^{\mathrm{T}},\ (\mathbf{T})_j=\left[(t_x)_j,(t_y)_j\right]^{\mathrm{T}},\quad j=1,2,\cdots,N$$

(7) 边界元方法(BEM)

分域建立离散方程：

基体：
$$\sum_{q=1}^{4}\left[\mathbf{H}_{pq}^{0}\mathbf{U}_{\Gamma_q}+\mathbf{G}_{pq}^{0}\mathbf{T}_{\Gamma_q}\right]+\mathbf{H}_{p0}^{0}\mathbf{U}_{\Gamma_0}+\mathbf{G}_{p0}^{0}\mathbf{T}_{\Gamma_0}=0,\quad p=0\sim 4$$

散射体：
$$\mathbf{H}^{1}\mathbf{U}_{\Gamma_0'}^{1}+\mathbf{G}^{1}\mathbf{T}_{\Gamma_0'}^{1}=0$$



考虑界面连接条件，得：
$$\begin{bmatrix}\mathbf{H}_{\mathrm{ex}}^{0} & \mathbf{G}_{\mathrm{ex}}^{0} & \mathbf{H}_{0}^{0} & \mathbf{G}_{0}^{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{H}^{1} & \mathbf{G}^{1}\end{bmatrix}\cdot\begin{bmatrix}\mathbf{U}_{\Gamma_e} & \mathbf{T}_{\Gamma_e} & \mathbf{U}_{\Gamma_0} & \mathbf{T}_{\Gamma_0}\end{bmatrix}^{\mathrm{T}}=0$$

考虑界面连接条件：
$$\mathbf{U}_{\Gamma_3}=e^{ik_x\cdot a}\mathbf{U}_{\Gamma_1},\quad \mathbf{U}_{\Gamma_4}=e^{ik_y\cdot a}\mathbf{U}_{\Gamma_2},$$
$$\mathbf{T}_{\Gamma_3}=-e^{ik_x\cdot a}\mathbf{T}_{\Gamma_1},\quad \mathbf{T}_{\Gamma_4}=-e^{ik_y\cdot a}\mathbf{T}_{\Gamma_2},$$

$$\begin{bmatrix}\mathbf{H}_{1}^{0}+e^{ik_x\cdot a}\mathbf{H}_{3}^{0} & \mathbf{H}_{2}^{0}+e^{ik_y\cdot a}\mathbf{H}_{4}^{0} & \mathbf{G}_{1}^{0}-e^{ik_x\cdot a}\mathbf{G}_{3}^{0} & \mathbf{G}_{2}^{0ik_y\cdot a}-\mathbf{G}_{4}^{0} & \mathbf{H}_{0}^{0} & \mathbf{G}_{0}^{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{H}^{1} & \mathbf{G}^{1}\end{bmatrix}\cdot\mathbf{X}=0$$

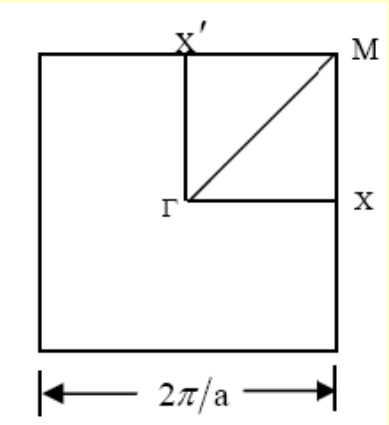
(7) 边界元方法(BEM)

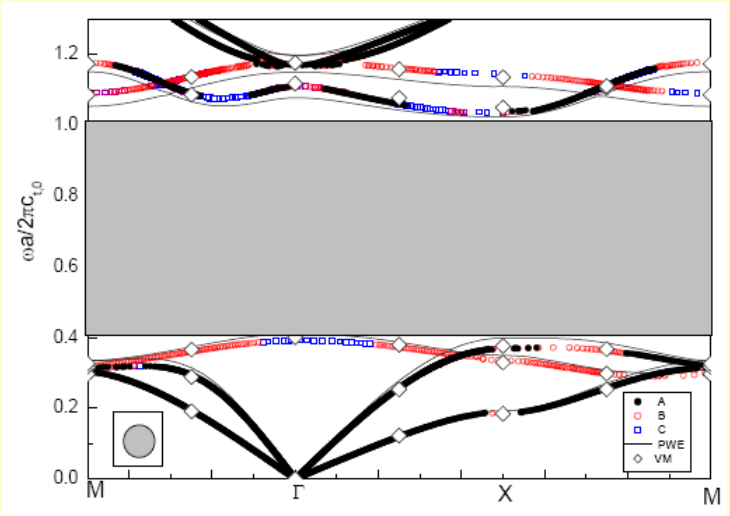
特征值方程：

$$\begin{bmatrix} \mathbf{H}_1^0 & \mathbf{H}_2^0 & \mathbf{G}_1^0 & \mathbf{G}_2^0 & \mathbf{H}_0^0 & \mathbf{G}_0^0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{H}^1 & \mathbf{G}^1 \end{bmatrix} \cdot \mathbf{X} = - \begin{bmatrix} e^{ik_x \cdot a}\mathbf{H}_3^0 & e^{ik_y \cdot a}\mathbf{H}_4^0 & -e^{ik_x \cdot a}\mathbf{G}_3^0 & -e^{ik_y \cdot a}\mathbf{G}_4^0 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \cdot \mathbf{X}$$

沿BZ区边界线性化： $\mathbf{AX} + \lambda \mathbf{BX} = 0$ $\lambda = e^{ik_x a}$ or $e^{ik_y a}$

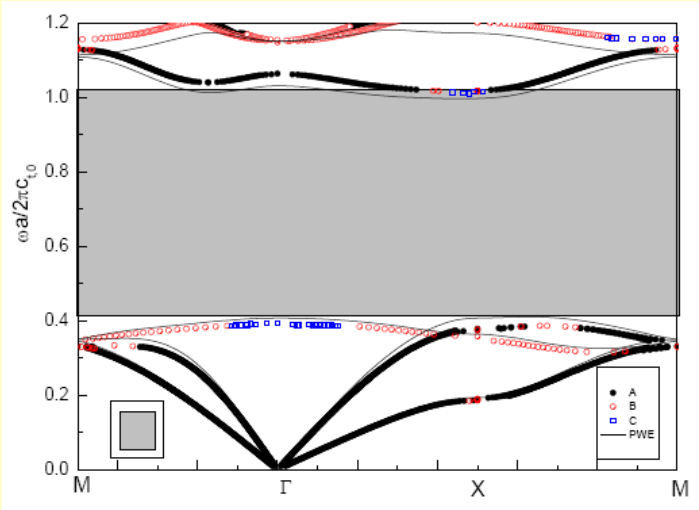
时 $\left(\left| |\lambda| - 1 \right| \le \varepsilon \right)$





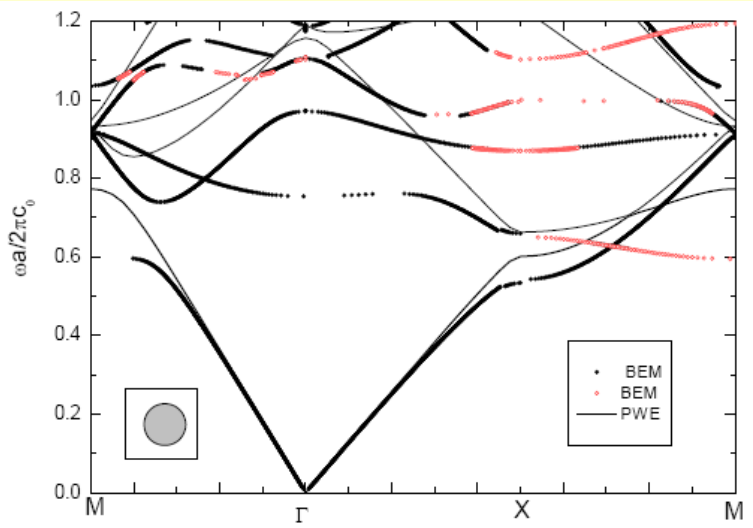
金/环氧, f=0.4

Li, et al. AEBE, 2012

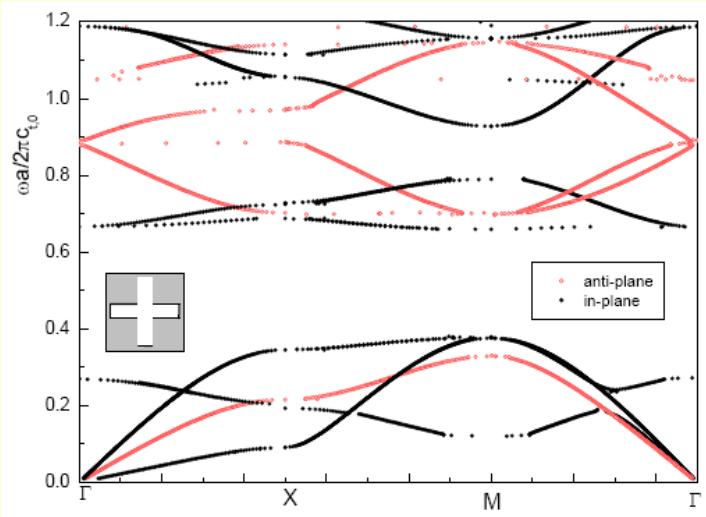


(7) 边界元方法(BEM)

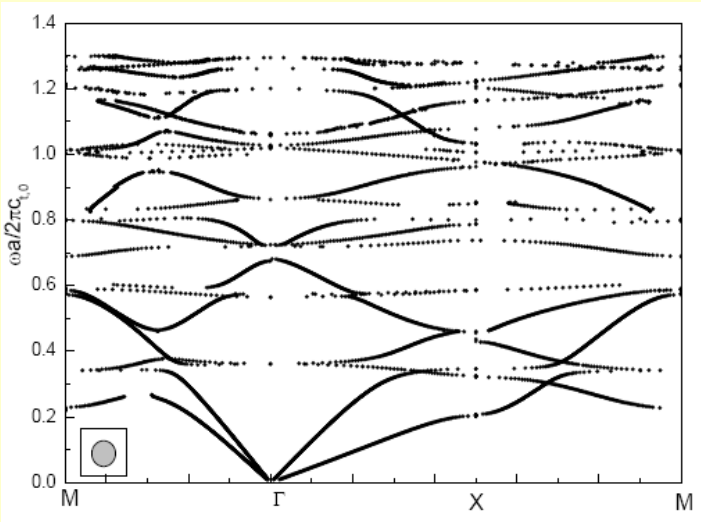
流固混合体系：



铝/汞



孔/铝



水/铁

Li, et al. WM, 2012

(7) 边界元方法(BEM)

方法二：

弹性动力学基本方程：

$$\nabla \cdot (\mathbb{C}(\mathbf{r}) : \nabla \mathbf{u}(\mathbf{r})) + \rho(\mathbf{r})\omega^2 \mathbf{u}(\mathbf{r}) = 0$$

$$\mathbf{u}(\mathbf{r}) = e^{i(\mathbf{k}\cdot\mathbf{r})}\mathbf{u}_{\mathbf{k}}(\mathbf{r}) \qquad \textbf{(Bloch theorem)}$$

$$(\nabla + i\mathbf{k}) \cdot [\mathbb{C}(\mathbf{r}) : (\nabla + i\mathbf{k}) \otimes \mathbf{u}_{\mathbf{k}}(\mathbf{r})] + \rho(\mathbf{r})\omega^2 \mathbf{u}_{\mathbf{k}}(\mathbf{r}) = 0$$

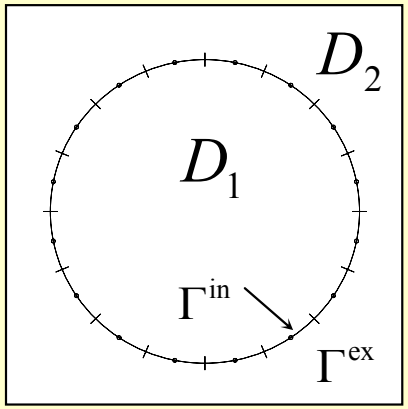
(7) 边界元方法(BEM)

Green函数:

— 级数形式:

$$G(\mathbf{r}-\mathbf{r}')=-\frac{i}{4}\sum_{m}H_0^{(1)}(k\,|\,\mathbf{r}-\mathbf{r}'-\mathbf{r}_m\,|)\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{a}}$$

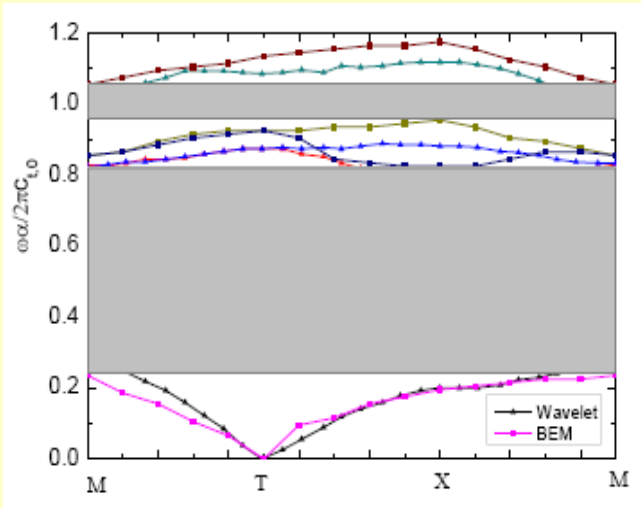
(反平面各向同性1D)



边界离散→ **BIE :**

(只需离散内边界 !)

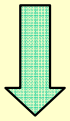
困难: **Green函数计算 !**



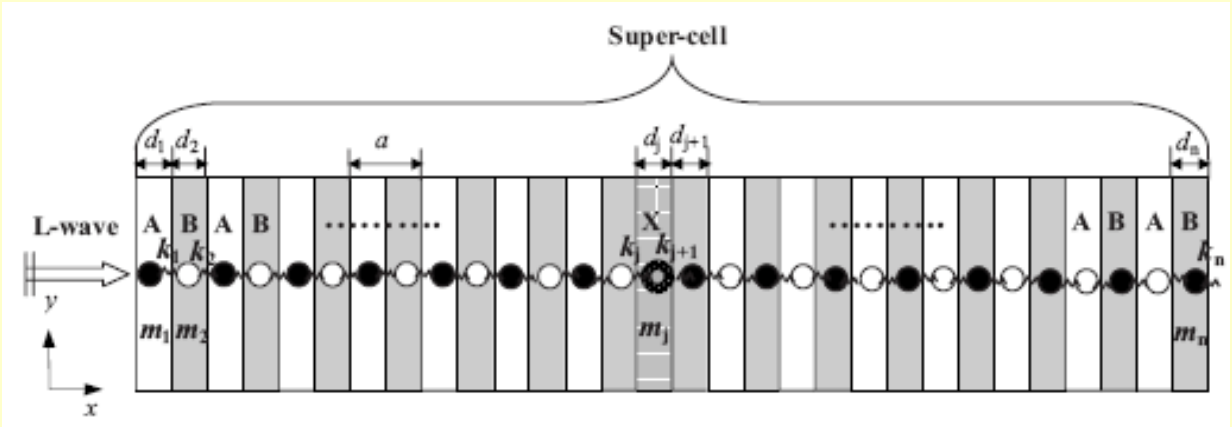
Li, et al. IEEE Ultra Symp. 2008 (Au/Epoxy)

(7) 集中质量法(LMM)

连续体



弹簧质量系统

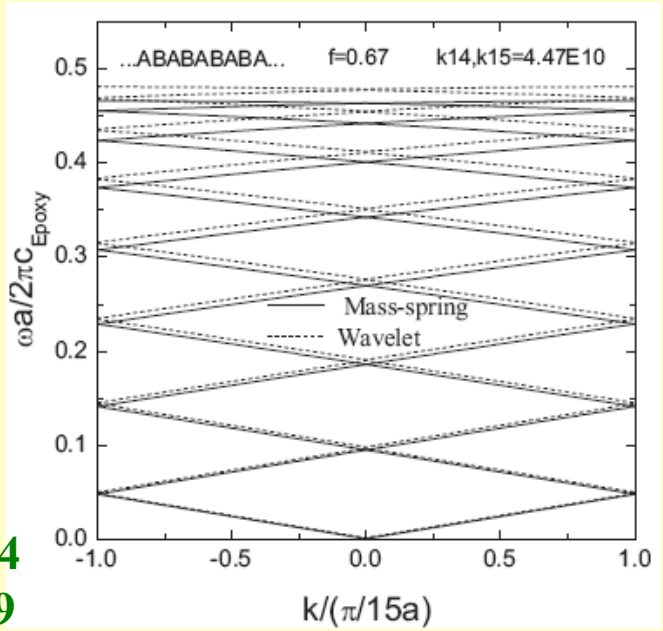


$$m_j \ddot{u}_j = k_j (u_{j+1} - u_j) - k_{j-1}(u_j - u_{j-1})$$

$$m_j = \rho_j S d_j$$

$$k_j = \frac{\left[2(\lambda_A + 2\mu_A)(\lambda_B + 2\mu_B)\right] \cdot S}{(\lambda_A + 2\mu_A) d_{j+1} + (\lambda_B + 2\mu_B) d_j}$$

$$\left(k_j = \frac{2\mu_A \mu_B S}{\mu_A d_{j+1} + \mu_B d_j} \right)$$



Wen, et al. APS, 2004
Yan, et al. APL, 2009

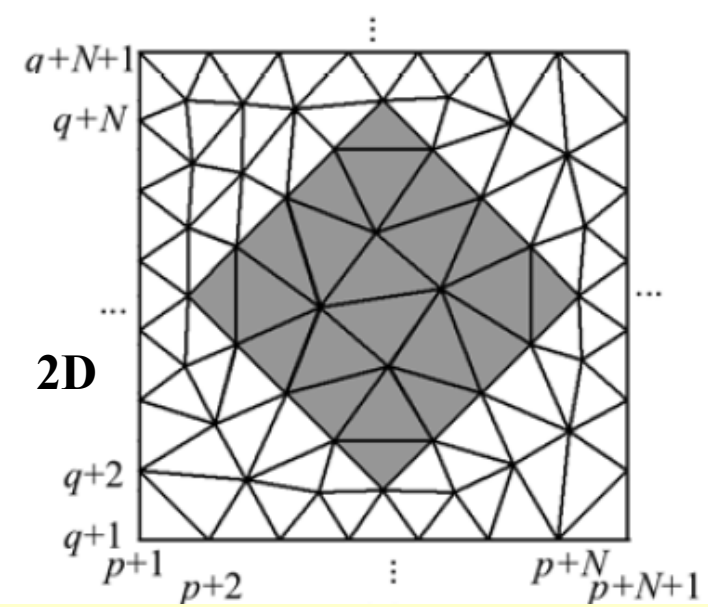
(7) 集中质量法(LMM)

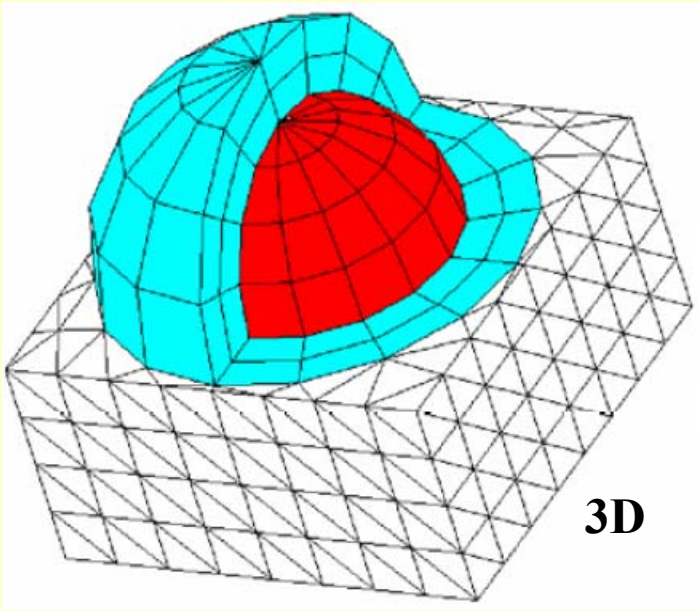
特点：

用于1维情况简单

用于2、3维情况复杂，计算量大

各种混合体系是否适用？





G. Wang, et al. PRB, 2004

其他方法???

已用于光子晶体带结构计算的其他方法:

Generalized multipole method

Moving least-square method

Multidomain pseudospectral method

The cell method

.....

可否用于声子晶体带结构的计算?

问题

- 3D系统(含缺陷系统)能带结构计算
- 表面波、Lamb波和弯曲波(缺陷态)能带结构计算
- 失谐和准周期系统的表征和计算模拟
- 能量耗散介质
- 非线性波
- 新材料的应用(压电/压磁/记忆/高弹/.....)
- 优化设计及制作
- 声功能器件方面的应用

本小组发表的部分论文

能带结构计算方法

1. Yan Z Z, Wang Y S. Wavelet-based method for calculating elastic band gaps of two-dimensional phononic crystals. *Physical Review* B, 2006, 74(22): 224303.
2. Yan Z Z, Wang Y S. Wavelet-based method for computing elastic band gaps of one-dimensional phononic crystals. *Science in China Series G: Physics Mechanics and Astronomy*, 2007, 50(5): 622-630.
3. Yan Z Z, Wang Y S, Zhang Ch. Wavelet method for calculating the defect states of two-dimensional phononic crystals. *Acta Mechanica Solida Sinica*, 2008, 21(2): 104-109.
4. Yan Z Z, Wang Y S. Calculation of band structures for surface waves in two-dimensional phononic crystals with a wavelet-based method. *Physical Review B*, 2008, 78(9): 094306.
5. Yan Z Z, Wang Y S, Zhang Ch. A method based on wavelets for band structure analysis of phononic crystals. *Computer Modeling in Engineering & Sciences*, 2008, 38(1): 59-87.
6. Su X X, Li J B, Wang Y S. A postprocessing method based on high-resolution spectral estimation for FDTD calculation of phononic band structures. *Physica B*, 2010, 405(10): 2444-2449.
7. Su X X, Wang Y S. A postprocessing method based on chirp Z transform for FDTD calculation of point defect states in two-dimensional phononic crystals. *Physica B*, 2010, 405(17): 3645-3649.
8. Su X X, Ma T X, Wang Y S. FDTD calculation of three-dimensional phononic band structures using a postprocessing method based on the filter diagonalization. *Physica Scripta*, 2011, 84(4): 045404.
9. Li F L, Wang Y S. Application of Dirichlet-to-Neumann map to calculation of band gaps for scalar waves in two-dimensional phononic crystals. *Acta Acoustics united with Acoustica*, 2011, 97(2): 284-290.
10. Li F L, Wang Y S, Zhang Ch. Bandgap calculation of two-dimensional mixed solid-fluid phononic crystals by Dirichlte-to-Neumann maps. *Physica Scripta*, 2011, 84(5): 055402.
11. Zhen N, Li F L, Wang Y S, Zhang Ch. Bandgap calculation for plane mixed waves in 2D phononic crystals based on Dirichlte-to-Neumann map. *Acta Mechanica Sinica*, 2012 (in press)
12. Li F L, Wang Y S, Zhang Ch. Boundary element method for bandgap computation of photonic crystals. *Optics Communications*, 2012, 285(5): 527-532.
13. Li F L, Wang Y S, Zhang Ch, Yu G L. Boundary element method for bandgap calculations of two-dimensional solid phononic crystals. *Engineering Analysis with Boundary Elements*, 2012 (in revise)
14. Li F L, Wang Y S, Zhang Ch, Yu G L. Bandgap calculations of two-dimensional solid-fluid phononic crystals with boundary element Method. *Wave Motion*, 2012 (in revise)
15. Li J B, Wang Y S, Zhang Ch. Dispersion relations of a periodic array of fluid-filled holes embedded in an elastic solid. *Journal of Computational Acoustics*, 2012, DOI No: 10.1142/S0218396X12500142 (published on-line)

本小组发表的部分论文

材料参数对带隙的影响

- **Zhou X Z, Wang Y S, Zhang Ch. Effects of material parameters on elastic band gaps of two-dimensional solid phononic crystals. *Journal of Applied Physics*, 2009, 106(1): 014903.**
- **Su X X, Wang Y F, Wang Y S. Effects of Poisson's ratio on band gaps and defect states in two-dimensional vacuum/solid porous phononic crystals. *Ultrasonics*, 2012, 52(2): 255-265.**
- **Ma T X, Wang Y S, Su X X, Wang Y F. Elastic band structures of two-dimensional solid phononic crystal with negative Poisson's ratios. *Physica B*, 2012 (published on-line)**

声子晶体板

- **Yao Z J, Yu G L, Wang Y S, Shi Z F. Point defect states of bending waves in phononic crystal thin plates. *International Journal of Solids and Structures*, 2009, 46(13): 2571-2576.**
- **Yao Z J, Yu G L, Wang Y S, Shi Z F, Li J B. Propagation of flexural waves in phononic crystal thin plates with linear defects. *Journal of Zhejiang University - Science A*. 2010, 11(10): 827-834.**

局域共振声子晶体

- **Yan Z Z, Zhang Ch, Wang Y S. Analysis of wave propagation and localization in periodic/disordered layered composite structures by a mass-spring model. *Applied Physics Letter*, 2009, 94(16): 161909.**
- **Wang Y F, Wang Y S, Su X X. Large bandgaps of two-dimensional phononic crystals with cross-like holes. *Journal of Applied Physics*, 2011, 110(11): 113520.**

纳米声子晶体

- **Chen A L, Wang Y S. Size-effect on band structures of nanoscale phononic crystals. *Physica E: Low-dimensional Systems and Nanostructures*, 2012, 41(1): 317-321.**
- **Zhen N, Wang Y S, Zhang Ch. Surface/interface effect on band structures of nanosized phononic crystals. *Mechanics Research Communications*, 2012 (in revise)**

本小组发表的部分论文

失谐和准周期声子晶体

- Chen A L, Wang Y S. Study on band gaps of elastic waves propagating in one dimensional disordered phononic crystals. *Physica B: Physics of Condensed Matter*, 2007, 392(1-2): 369-378.
- Chen A L, Wang Y S, Guo Y F, Wang Z D. Band structures of Fibonacci phononic quasicrystals. *Solid State Communications*, 2008, 145(3): 103-108.
- Chen A L, Wang Y S, Yu G L, Guo Y F, Wang Z D. Elastic wave localization in two-dimensional phononic crystals with one-dimensional quasi-periodicity and random disorder. *Acta Mechanica Solida Sinica*, 2008, 21(6): 517-528.
- Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Wave localization in two-dimensional periodic systems with randomly disordered size. *European Physical Journal B*, 2009, 67(4): 501-505.
- Yan Z Z, Zhang Ch, Wang Y S. Attenuation and localization of bending waves in a periodic/disordered fourfold composite beam. *Journal of Sound and Vibration*. 2009, 327(1-2): 109-120.
- Chen A L, Wang Y S, Li J B, Zhang Ch. Localization of elastic waves in two-dimensional randomly disordered solid phononic crystals. *Waves in Random and Complex Media*, 2010, 20(1): 104-121.
- Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Wave localization in randomly disordered layered three-component phononic crystals with thermal effects. *Archive of Applied Mechanics*, 2010, 80(6): 629-640.
- Yan Z Z, Zhang Ch, Wang Y S. Wave propagation and localization in randomly disordered layered composites with local resonances. *Wave Motion*, 2010, 47(7): 409-420.
- Yan Z Z, Zhang Ch, Wang Y S. Elastic wave localization in two-dimensional phononic crystals with one-dimensional random disorder and aperiodicity. *Physica B*, 2011, 406(5): 1154-1161.
- Chen A L, Wang Y S, Zhang Ch. Wave propagation in one-dimensional solid-fluid quasi-periodic and aperiodic phononic crystals. *Physica B*, 2012, 407(3): 324-329.

本小组发表的部分论文

压电声子晶体（周期或失谐）

- Li F M, Wang Y S. Study on wave localization in disordered periodic layered piezoelectric composite structures. *International Journal of Solids and Structures*, 2005, 42(24-25): 6457-6474.
- Li F M, Wang Y S, Chen A L. Wave localization in randomly disordered periodic piezoelectric rods. *Acta Mechanica Solida Sinica*, 2006, 19(1): 50-57.
- Li F M, Wang Y S. Study on localization of plane elastic waves in disordered periodic 2-2 piezoelectric composite structures. *Journal of Sound and Vibration*, 2006, 296(3): 554-566.
- Li F M, Xu M Q, Wang Y S. Frequency-dependent localization length of SH-wave in randomly disordered piezoelectric phononic crystals. *Solid State Communications*, 2007, 141(5): 296-301.
- Chen A L, Li F M, Wang Y S. Localization of flexural waves in a disordered periodic piezoelectric beam. *Journal of Sound and Vibration*, 2007, 304(3-5): 863-874.
- Li F M, Wang Y Z, Fang B, Wang Y S. Propagation and localization of two-dimensional in-plane elastic waves in randomly disordered layered piezoelectric phononic crystals. *International Journal of Solids and Structures*, 2007, 44(22-23): 7444-7456
- Wang Y Z, Li F M, Huang W H, Wang Y S. Effects of inclusion shapes on the band gaps in two-dimensional piezoelectric phononic crystals. *Journal of Physics: Condensed Matter*, 2007, 19(49): 496204.
- Wang Y Z, Li F M, Huang W H, Wang Y S. The propagation and localization of Rayleigh waves in disordered piezoelectric phononic crystals. *Journal of the Mechanics and Physics of Solids*, 2008, 56(4): 1578-1590.
- Li J Q, Li F M, Wang Y S, Kishimoto K. Wave propagation in two-dimensional disordered piezoelectric phononic crystals. *Acta Mechanica Solida Sinica*, 2008, 21(6): 507-516.
- Wang Y Z, Li F M, Wang Y S, Kishimoto K, Huang W H. Tuning of band gaps for a two-dimensional piezoelectric phononic crystal. *Acta Mechanica Sinica*, 2009, 25(1): 65-71.
- Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Wave Band gaps in three-dimensional periodic piezoelectric structures, *Mechanics Research Communications*, 2009, 36(4): 461-468.
- Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Wave localization in randomly disordered periodic piezoelectric rods with initial stress. *Acta Mechanica Solida Sinica*, 2008, 21(6): 523-535.
- Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Band gaps of elastic waves in three-dimensional piezoelectric phononic crystals with initial stress. *European Journal of Mechanics - A/Solids*, 2010, 29(2): 182-189.

本小组发表的部分论文

压电/压磁声子晶体

- **Wang Y Z, Li F M, Huang W H, Jiang X, Wang Y S, Kishimoto K. Wave band gaps in two-dimensional piezoelectric/piezomagnetic phononic crystals, *International Journal of Solids and Structures*, 2008, 45(14-15): 4203-4210.**
- **Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Elastic wave band gaps in magnetoelectroelastic phononic crystals. *Wave Motion*, 2009, 46(1): 47-56.**
- **Wang Y Z, Li F M, Kishimoto K, Wang Y S, Huang W H. Band gap behaviors of periodic magnetoelectroelastic composite structures with Kagome lattices. *Waves in Random and Complex Media*, 2009, 19(3): 509-520.**
- **Pang Y, Wang Y S, Liu J X, Fang D N. Study on band structures of elastic wave propagating in piezoelectric/piezomagnetic layered periodic structures. *Smart Materials and Structures*, 2010, 19(5): 055012.**