

材料宏观力学行为-HW1

姓名 张家瑞 学号 2401111734 院系 工学院力学与工程科学系

1 晶体结构部分

1.1 简述晶体结构 (crystal structure) 和点阵 (lattice) 的区别？

晶体结构的概念是包含基元和点阵的，点阵与基元结合后的实际原子排列成为晶体结构；而点阵是几何空间中的周期性排列规律，表现的是晶体结构中原子的规则排列。

1.2 Why no face-centered structures in the tetragonal system?

对于四方晶系 (tetragonal)，其特点是 $a = b \neq c$ ， $\alpha = \beta = \gamma = 90^\circ$ 。其需要满足四重旋转对称性。而对于面心四方晶系无法独立存在，因为它要么因对称性过高被归入立方晶系，要么因对称性不足而被重新定义为体心四方或简单四方结构。

1.3 确定下图斜面的晶面指数。

六方晶系晶面指数是晶面在晶轴上的截距的倒数比值，图中的斜面与四轴的截距分别为 1、1、-0.5、1，因此晶面指数为 $(11\bar{2}1)$ 。

1.4 对于面心立方或体心立方点阵，则其最大面间距的面是什么？写出该面间距表达式。

最大面间距的面是密排面。对于面心立方，最大间距面为 (111)，面间距为 $a/\sqrt{3}$ ；对于体心立方，最大间距面为 (110)，面间距为 $a/\sqrt{2}$ ；

1.5 用 objective structure 框架表示下图中 armchair 型碳纳米管结构。

我们考虑使用 Group C 来描述 armchair 型碳纳米管结构，分为操作 h 与 g ， h 为绕着对称轴的旋转加平移， g 为绕着对称轴的旋转。

假设原子半径为 a ，我们考虑两个相邻的原子，在垂直于对称轴的截平面上，共有 6 对原子，则在 g 算符中，每次绕着对称轴旋转的角度为 $\pi/3$ ，即 $\psi = \pi/3$ ；对于平移加旋转的操作，需要进行 12 次操作才能绕着对称轴旋转一周，且每次沿着对称轴平移的距离为 $2a * \cos \pi/6 = \sqrt{3}a$ ，即 $\theta = \pi/6$ ， $\tau = \sqrt{3}a$ 。

为 $h^p g^q : p \in \mathbb{Z}, q = 1, \dots, n$ ，其中 $h = (\mathbf{R}_\theta | \tau \mathbf{e} + ((\mathbf{R}_\theta - \mathbf{I})x_0)$ ， $g = (\mathbf{R}_\psi | (\mathbf{R}_\psi - \mathbf{I})x_0)$ ， $\theta = \pi/6$ ， $\tau = \sqrt{3}a$ ， $\psi = \pi/3$ 。

材料宏微观力学行为 - HW2

张家瑞 2401111734

1. 推导 Kelvin 问题的格林函数解，并基于此推导无限弹性空间中偶极子引起的位移场方程。

1. 具有体力 \vec{f} 的弹性力学方程为

$$\mathcal{L}\vec{u} = -\frac{1}{\mu}\vec{f}$$

设上述方程的解具有 P-N 形式，即

$$\vec{u} = \psi - \frac{1}{\mathcal{L}(1-\nu)}\nabla(\psi_0 + r\psi)$$

整理，计算得

$$\nabla^2\psi - \frac{1}{2\mathcal{L}(1-\nu)}\nabla(\nabla^2\psi_0 + r\nabla^2\psi) = -\frac{1}{\mu}\vec{f}$$

设 ψ 与 ψ_0 分别满足 $\nabla^2\psi = -\frac{1}{\mu}\vec{f}$ 、 $\nabla^2\psi_0 = \frac{1}{\mu}\vec{f}\cdot\vec{f}$

$$\text{则有一个解为 } \begin{cases} \psi = \frac{1}{4\pi\mu} \iiint_{\mathcal{R}} \frac{f(x,y,z)}{\rho} d\xi d\eta d\zeta \\ \psi_0 = -\frac{1}{4\pi\mu} \iiint_{\mathcal{R}} \frac{\vec{f}\cdot\vec{f}(x,y,z)}{\rho} d\xi d\eta d\zeta \end{cases}$$

其中 $\rho = \sqrt{(x-\xi)^2 + (y-\eta)^2 + (z-\zeta)^2}$ ， $\vec{z} = \xi\vec{i} + \eta\vec{j} + \zeta\vec{k}$ 。

$$\text{则有 } \vec{u} = \frac{1}{16\pi\mu(1-\nu)} \left[\mathcal{L}(3-4\nu) \iiint_{\mathcal{R}} \frac{\vec{f}}{\rho} d\tau_3 + \iiint_{\mathcal{R}} \frac{\vec{f}\cdot\vec{f}}{\rho^3} \vec{\rho} d\tau_3 \right]$$

其中 $\vec{\rho} = \vec{r} - \vec{z} = (x-\xi)\vec{i} + (y-\eta)\vec{j} + (z-\zeta)\vec{k}$ ， $d\tau_3 = d\xi d\eta d\zeta$ 。

当体力 \vec{f} 为集中力时，记为 \vec{F} ，作用点为 $\vec{r}_0 = (x_0, y_0, z_0)$ 。

$$\text{则有 } \vec{u} = \frac{1}{16\pi\mu(1-\nu)} \left[\mathcal{L}(3-4\nu) \frac{\vec{F}}{R} + \frac{\vec{R}\cdot\vec{F}}{R^3} \vec{R} \right]$$

其中 $\vec{R} = \vec{r} - \vec{r}_0 = (x-x_0)\vec{i} + (y-y_0)\vec{j} + (z-z_0)\vec{k}$ 。

对于单位强度的力偶极子, 力方向为 $\pm z$.

$$u_i^{dp}(\vec{r}) = P G_{iz}(x, y, z - \Delta z/2) - P G_{iz}(x, y, z + \Delta z/2) \\ = -(G_{iz}(x, y, z + \Delta z/2) - G_{iz}(x, y, z - \Delta z/2)) / \Delta z$$

随着 $\Delta z \rightarrow 0$, 有 $u_i^{dp}(\vec{r}) = -\frac{\partial}{\partial z} G_{iz}(\vec{r})$

$$= \frac{1-2\nu}{8\pi\mu(1-\nu)} \frac{x_i}{r^3} = \frac{1+\nu}{12\pi(1+\nu)B} \frac{x_i}{r^3}.$$

2. 推导不同材料的 misfitting sphere problem: 其中 ΔV 为外球 B 夹杂前后外球体积变化, Δv 为夹杂前后内孔体积变化. 夹杂体模量角标为 A.

$$\Delta V_{int} \equiv \Delta V - \Delta v, \\ \Delta V_{int} = \Delta v \frac{4}{3}\mu_A \left(\frac{1}{B_A} - \frac{1}{B_B} \right) \left(1 + \frac{4\mu_A}{3B_B} \right)^{-1}$$

2. 对于 misfitting sphere 问题, 有 $\Delta V = \Delta V_A + |\Delta V_B|$

其中 ΔV_A 为孔洞扩大的体积, ΔV_B 为球体压缩的体积.

且由 $\sigma_{rr}^A = -\frac{\mu_A \Delta v}{\pi r^3}$

$$\sigma_{rr}^B = -p_B = +B_B \epsilon_B = -B_B \frac{|\Delta V_B|}{\frac{4}{3}\pi r^3}.$$

由 $\sigma_{rr}^A = \sigma_{rr}^B \quad \therefore$ 有 $|\Delta V_B| = \left(\frac{4\mu_A}{3B_B} \right) \Delta V_A$

$$\therefore \Delta V = \Delta V_A \left(1 + \frac{4\mu}{3B} \right)$$

又由于 $\Delta V_{int} = \Delta V - \Delta v = 0$ (内力不引起体积变化)

则有象流体压力 $-p^z = \frac{1}{3}(\sigma_{rr}^z + \sigma_{\theta\theta}^z + \sigma_{\phi\phi}^z) = B(\epsilon_{rr}^z + \epsilon_{\theta\theta}^z + \epsilon_{\phi\phi}^z) = \frac{\mu \Delta v}{\pi r^3}$

又由 $\Delta V = \Delta V_A \left(1 + \frac{4\mu}{3B} \right)$

$$\therefore \Delta V_{int} = \Delta V - \Delta v = \Delta V_A \left(1 + \frac{4\mu}{3B_A} \right) - \Delta v = \Delta v \left(1 + \frac{4\mu}{3B_B} \right)^{-1} \left(1 + \frac{4\mu}{3B_A} \right) - \Delta v \\ = \Delta v \frac{4}{3}\mu_A \left(\frac{1}{B_A} - \frac{1}{B_B} \right) \left(1 + \frac{4\mu_A}{3B_B} \right)^{-1}.$$

3. 推导一维谐振子的熵。

$$S \approx k_B \ln \frac{k_B T}{h\nu}.$$

3. 温度 T 的一维简谐振动模型, 设质量 m , 弹簧刚度 k , 有系统能量 $E(x, p) = \frac{1}{2} kx^2 + \frac{p^2}{2m}$.

又由量子力学中的不确定性 $\Delta x \Delta p < h$, 其中 h 为普朗克常数.

$$\begin{aligned} \text{有 } Z &= \frac{1}{h} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp \exp\left(-\frac{kx^2}{2k_B T} - \frac{p^2}{2mk_B T}\right) \\ &= \frac{1}{h} \sqrt{\frac{2\pi k_B T}{k}} \sqrt{2\pi mk_B T} \\ &= \frac{k_B T}{h\nu}. \end{aligned}$$

其中 $\nu = \frac{1}{2\pi} \sqrt{k/m}$ 为振动频率

因此有亥姆霍兹自由能 $F = -k_B T \ln Z = -k_B T \ln \frac{k_B T}{h\nu}$.

∴ 有能量 $E = k_B T$.

因此系统熵为 $S = \frac{E-F}{T} = k_B \left(1 + \ln \frac{k_B T}{h\nu}\right)$

而当温度足够高, 有 $k_B T \gg h\nu$.

∴ 有 $S \approx k_B \ln \frac{k_B T}{h\nu}$.

4.

A sample of FCC platinum is held at $T = 2000$ K, just below its melting temperature for a long period of time so that vacancy equilibrium is established.

- (a) Calculate the equilibrium concentration of vacancies (in units of vacancies per m^3) when no external pressure is acting on the solid.
- (b) Now consider the effects of imposing an external pressure, p_{ext} , onto the solid at the temperature of 2000 K. Calculate the pressure needed to reduce the vacancy concentration to 1% of the value found in (a).

The lattice and vacancy quantities needed for these calculations are given in Tables A.1 and C.1.

Element	Atomic number	Ω (\AA^3)	r_0 (\AA)
Pt	78	15.10	1.534

Table C.1. Properties of vacancies in pure metals [26]. $\chi_v(T_m)$: vacancy fraction at the melting temperature (in 10^{-3}). Δs_v : activation entropy of formation (in units of k_B). Δh_v : activation enthalpy of formation (in eV). ΔV_v^{rlx} : relaxation volume of the vacancy (in units of atomic volume Ω). Δh_v^m : activation enthalpy of migration (in eV). R stands for rhombohedral crystal structure. T stands for tetragonal crystal structure. BCT stands for body-centered tetragonal crystal structure. Para and ferro stand for the paramagnetic and ferromagnetic phases of iron (Fe), respectively.

Element	Structure	$\chi_v(T_m)$	Δs_v	Δh_v	ΔV_v^{rlx}	Δh_v^m
Pt	FCC	9.4	0.4	1.35 ± 0.05	-0.28	1.43 ± 0.05

4. 解: 在没有外部压力的

铂的空位浓度为

$$C = \exp\left(-\frac{\Delta h_v(1.62e-19) - T\Delta s_v \cdot R_B}{k_B T}\right)$$

由于 $\Delta h_v = 1.35$

$$\Delta s_v = 0.4$$

$$R_B = 1.38e-23$$

∴ 有 $C = 5.4 \times 10^{-4}$.

因为 $\Delta V_0^{rlx} = \Delta V_0 - \Omega$.



又由于有外力的情况下, 有 $C' = C \exp\left(-\frac{p\Delta V_0^{rlx} \Omega + p\Omega}{k_B T}\right)$

而 $\Omega = 15.1 \times 10^{-30} m^3$

$\Delta V_0^{rlx} = -0.28$, $\Delta V_0 = 1 - 0.28$

由 $C' = 1\% \cdot C$ ∴ 有 $p = \frac{k_B \cdot T \cdot \ln 0.01}{-\Delta V_0 \cdot \Omega}$

$= 1.177 \times 10^{10} Pa = 11.77 MPa$

5.

A long wire of pure Au is held at room temperature for a very long time so that equilibrium is established. The length of the wire in this state is L_0 . Then the wire is heated to $T_1 = 900^\circ\text{C}$ and held for a sufficiently long time to establish equilibrium at that temperature, before being quenched instantaneously to room temperature. The length of the wire in the quenched state is L_q .

- (a) Write an expression for L_q/L_0 as a function of T_1 and the thermodynamic properties of vacancies in Au, which are given in Table C.1.
 (b) The quenched wires are heated to a slightly elevated temperature, T , and annealed for a time, t , before being cooled again to room temperature where the length of the wire, L , is again measured. Write an expression showing how the length of the wire would be expected to change with increasing annealing time. You may assume that the equilibrium vacancy concentration at the annealing temperature T is so small that it can be ignored.

Element	Structure	$\chi_v(T_m)$	Δs_v	Δh_v	ΔV_v^{int}	Δk_v^{eq}
Ag	FCC	1.7	1.5	1.11 ± 0.05		0.66 ± 0.05
Al	FCC	9.4	0.7	0.67 ± 0.03	-0.05	0.61 ± 0.03
Au	FCC	7.2	0.72	0.93 ± 0.04	-0.15	0.71 ± 0.05

(b) 由于扩散方程有 $\frac{L(t) - L_0}{L_q - L_0} = \exp(-\frac{t}{\tau})$. 其中 $\tau = \exp(\frac{\Delta h_v^{\text{eq}}}{k_B T})$
 有 $L(t) = L_0 + (L_q - L_0) \exp(-\frac{t}{\tau})$.

(a) 由于 $\Delta V_v^{\text{int}} = -0.15 \text{ eV}$

$$\Delta S_v = 0.72 k_B$$

$$\chi_v = \exp\left(\frac{\Delta S_v}{k_B}\right) \exp\left(-\frac{\Delta h_v}{k_B T}\right) \left(\frac{\Delta V_v}{\Omega}\right)$$

$$\text{且 } \frac{L_q - L_0}{L_0} = \frac{\Delta L}{L}$$

$$\text{又由 } \frac{\Delta L}{L} = \frac{1}{2} \chi_v$$

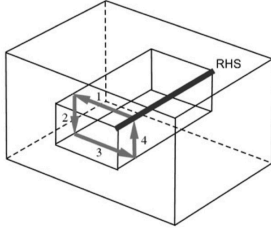
$$\therefore \text{有 } \frac{L_q}{L_0} = 1 + \frac{1}{2} \exp\left(\frac{\Delta S_v}{k_B}\right) \exp\left(-\frac{\Delta h_v}{k_B T}\right) \left(\frac{\Delta V_v}{\Omega}\right)$$

$$\therefore L_q/L_0 = 1 + 0.582 e^{-10917/T}$$

材料宏观力学行为 - HW3

张家瑞 2401111734

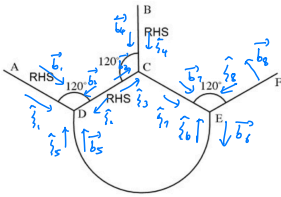
1. 一条右手螺位错依次在平面 1, 2, 3, 4 上滑移。描述该螺位错滑移 100 周以后, 整体形状变成了什么?



整体形状会形成一个螺旋管状体。

整体会形成一个以位错线为中心轴, 沿着位错滑移方向推进的螺旋形体。

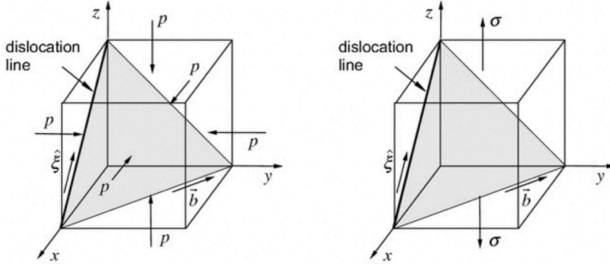
2. 确定 EF 位错的 Burgers 矢量, 位错类型, 写出分析过程。



由于 AD、CD、BC 均为 RHS, 可知 DE 在 D 点, CE 在 C 点也均为 RHS, 由于 DE 为形成位错环, 有在 E 点为 LHS. 而 CE 在 E 点为 RHS.

∴ 有 EF 为纯刃位错, 且伯格斯矢量为 \vec{b} , 方向如 \vec{b}_8 所示.

3. 计算位错线受力



由于位错线受力 $\vec{f} = (\vec{b} \cdot \vec{\sigma}) \times \hat{\xi}$

图1: 由图可知, $\vec{b} = b \frac{1}{\sqrt{2}} [\bar{1} 1 0]$ $\hat{\xi} = \frac{1}{\sqrt{2}} [\bar{1} 0 1]$

$$\vec{\sigma} = \begin{bmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{bmatrix}$$

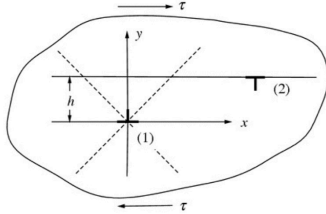
$$\begin{aligned} \therefore \text{有 } \vec{f} &= b \frac{1}{\sqrt{2}} [p \ -p \ 0] \times \frac{1}{\sqrt{2}} [\bar{1} \ 0 \ 1] \\ &= -\frac{bp}{2} [1 \ 1 \ 1] \end{aligned}$$

图2: 由图可知, $\vec{b} = b \frac{1}{\sqrt{2}} [\bar{1} 1 0]$ $\hat{\xi} = \frac{1}{\sqrt{2}} [\bar{1} 0 1]$

$$\vec{\sigma} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma \end{bmatrix}$$

$$\begin{aligned} \therefore \text{有 } \vec{f} &= b \frac{1}{\sqrt{2}} [0 \ 0 \ 0] \times \frac{1}{\sqrt{2}} [\bar{1} \ 0 \ 1] \\ &= [0 \ 0 \ 0] \end{aligned}$$

4. 位错 1 在原点，位错 2 最初在无穷远处，距 x 轴距离 h，求临界 shear stress，可以从位错 1 上方 glide 通过。



4. 解: 由 $f_x^{int} = \sigma_{xy}^{(1)} b_x^{(2)} = \frac{\mu b_x^{(1)} b_x^{(2)}}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2} = \frac{\mu b_x^{(1)} b_x^{(2)}}{2\pi(1-\nu)} \frac{x(x^2-h^2)}{(x^2+h^2)^2}$

对于位错 (2) 需要的力: $f_x^{app} = \tau b_x^{(2)}$

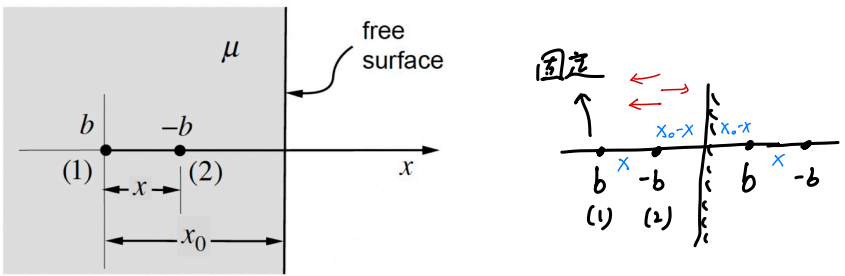
因此 $f_x^{int} + f_x^{app} = 0$

$$\therefore \frac{\mu b_x^{(1)} b_x^{(2)}}{2\pi(1-\nu)} \frac{x(x^2-h^2)}{(x^2+h^2)^2} + \tau b_x^{(2)} = 0$$

$$\therefore \tau = - \frac{\mu b_x^{(1)}}{2\pi(1-\nu)} \frac{x(x^2-h^2)}{(x^2+h^2)^2}$$

$$= - \frac{\mu b_x^{(1)}}{2\pi(1-\nu)h} \frac{\beta(\beta^2-1)}{(\beta^2+1)^2}$$

5. 两条方向相反的螺位错，位错 1 位置固定。位错 2 可沿着 x 轴滑移。求临界位置 $x = x_c$ ，使得位错 2 平衡。



对于图中，沿着 x 方向分布的螺位，位错之间相互作用 $f = \frac{\mu b^{(1)} b^{(2)}}{2\pi r}$

考虑 imaginary space.

$$\text{有 } \frac{1}{x} + \frac{1}{2x_0 - x} = \frac{1}{2x_0 - 2x} \quad \Rightarrow \quad x^2 - 6x_0 \cdot x + 4x_0^2 = 0$$

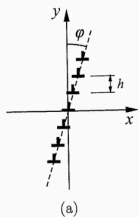
解得 $x = (3 - \sqrt{5})x_0$

材料宏观力学行为 - HW4

张象瑞 2401111734

1.

Consider an infinite periodic array of edge dislocations with Burgers vector b . As shown in Fig. 14.22a, the array is oriented at an angle φ with respect to the y axis. The spacing between the adjacent glide planes of the dislocations is h . Obtain an expression of the stress field of the dislocation array in the limit of $x \rightarrow \pm\infty, y = 0$.



解: 对于一个沿 x, y 方向均有分量的刃位错, 其产生的应力场为

$$\sigma_{xy}(x, y) = \frac{\mu}{2\pi(1-\nu)r^2} [b_x x (1 - \frac{2y^2}{r^2}) - b_y y (1 - \frac{2x^2}{r^2})]$$

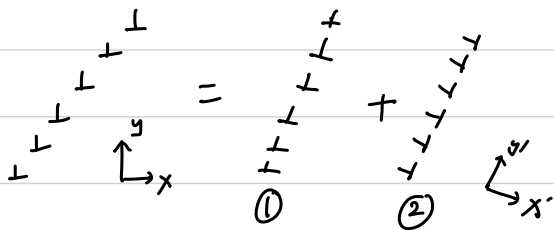
$$\sigma_{yy}(x, y) = \frac{\mu}{2\pi(1-\nu)r^2} [b_x y (1 - \frac{2y^2}{r^2}) + b_y x (1 + \frac{2y^2}{r^2})]$$

$$\sigma_{xx}(x, y) = \frac{-\mu}{2\pi(1-\nu)r^2} [b_x y (1 + \frac{2x^2}{r^2}) + b_y x (1 - \frac{2x^2}{r^2})]$$

对于沿着 y 方向周期 h 的刃位错引起的应力场

$$\sigma_{ij}^{yPBC}(x, y) = \sum_{n=-\infty}^{\infty} \sigma_{ij}(x, y - nh)$$

又由于图示位错可分为两部分的共同影响, 即



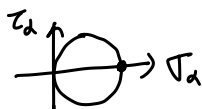
而 (1) 在 $x' \rightarrow \pm\infty, y \rightarrow 0$ 处的

$$\sigma_{xx}, \sigma_{yy}, \sigma_{xy} \text{ 均为 } 0$$

(2) 在 $x' \rightarrow \pm\infty, y \rightarrow 0$ 处的

$$\sigma_{xx}, \sigma_{yy} \text{ 为 } 0, \quad \sigma_{xy} = \frac{\text{sgn}(x)\mu b}{(1-\nu)h}$$

因此产生的应力场为主方向沿着与 y 轴夹角 φ , 大小为 $\frac{\text{sgn}(x)\mu b}{(1-\nu)h}$.



经换算 $x-y$ 坐标系后为:

$$\sigma_{xx} = \frac{\text{sgn}(y)\mu b}{2(1-\nu)h} \cdot (1 - \cos\varphi)$$

$$\sigma_{yy} = \frac{\text{sgn}(y)\mu b}{2(1-\nu)h} (1 + \cos\varphi)$$

$$\sigma_{xy} = \frac{\text{sgn}(x)\mu b}{2(1-\nu)h} \cdot \sin\varphi$$

2.

Figure 14.27 shows a tilt boundary containing a macroscopic step. Let the misorientation between the two crystals be θ . Construct a dislocation model for the three straight sections of the tilt boundary and determine their dislocation content. Explain why this boundary does not have a long-range ($1/r$) stress field, contrary to the stepped boundary shown in Fig. 14.16d.

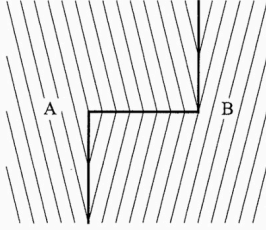


Figure 14.27. A non-straight tilt boundary (thick lines) separating crystal A and crystal B. The thin lines indicate the orientation of atomic planes in the two crystals.

在该问题中，这是其中台阶的形成引入了位错的不连续性，其中水平部分可能不为纯的刃位错。进而使得产生的应力均互相抵消。边界未出现长程应力场。而在 14.16d 中，是由于单个刃位错的滑移形成的。