

Assignment #5 Solutions:

Independently by

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Problem 5.1)

$$a) \quad U(x) = C_2 x^2 - C_3 x^3 - C_4 x^4$$

Assume the system satisfies Boltzmann Statistics.

Hence, the expectation value of x is following.

$$\begin{aligned} \langle x \rangle &= \frac{\int_{-\infty}^{\infty} x \cdot e^{-\frac{U(x)}{k_B T}} dx}{\int_{-\infty}^{\infty} e^{-\frac{U(x)}{k_B T}} dx} \quad , \quad \text{Let } \beta = \frac{1}{k_B T} \\ &= \frac{\int_{-\infty}^{\infty} x \cdot e^{-\beta U(x)} dx}{\int_{-\infty}^{\infty} e^{-\beta U(x)} dx} \end{aligned}$$

Let's assume x is small. C_2 is the dominant term.

Therefore, C_3 and C_4 have relatively small contributions.

We take the Taylor expansion of C_3 and C_4 terms.

$$\begin{aligned} \langle x \rangle &= \frac{\int_{-\infty}^{\infty} x(1 + \beta C_3 x^3 + \beta C_4 x^4 + \dots) e^{-\beta C_2 x^2} dx}{\int_{-\infty}^{\infty} (1 + \beta C_3 x^3 + \beta C_4 x^4 + \dots) e^{-\beta C_2 x^2} dx} \\ &\approx \frac{\int_{-\infty}^{\infty} (x + \beta C_3 x^4 + \beta C_4 x^5) e^{-\beta C_2 x^2} dx}{\int_{-\infty}^{\infty} (1 + \beta C_3 x^3 + \beta C_4 x^4) e^{-\beta C_2 x^2} dx} \end{aligned}$$

$$\text{Note : } \int_{-\infty}^{\infty} x e^{-\beta C_2 x^2} dx = \int_{-\infty}^{\infty} \beta C_4 x^5 e^{-\beta C_2 x^2} dx = 0$$

$$\int_{-\infty}^{\infty} \beta C_3 x^3 e^{-\beta C_2 x^2} dx = 0$$

Problem 5.1)

a) Continued. $\langle x \rangle \approx \frac{\int_{-\infty}^{\infty} \beta C_3 x^4 e^{-\beta C_2 x^2} dx}{\int_{-\infty}^{\infty} (1 + \beta C_4 x^4) e^{-\beta C_2 x^2} dx}$

Now we only need to evaluate the two integrals.

$$\int_{-\infty}^{\infty} \beta C_3 x^4 e^{-\beta C_2 x^2} dx, \quad \text{Let } \beta C_2 x^2 = y$$

$$x^2 = \frac{y}{\beta C_2}, \quad x = \frac{\sqrt{y}}{\sqrt{\beta C_2}}$$

$$dx = \frac{1}{\sqrt{\beta C_2}} \cdot \frac{dy}{\sqrt{y}}$$

$$= 2 \int_0^{\infty} \beta C_3 x^4 e^{-\beta C_2 x^2} dx$$

$$= 2 \int_0^{\infty} \beta C_3 \cdot \frac{y^2}{\beta^2 C_2^2} e^{-y} \cdot \frac{1}{\sqrt{\beta C_2}} \cdot \frac{dy}{\sqrt{y}}$$

$$= 2 \beta C_3 \cdot \frac{1}{(\beta C_2)^{\frac{5}{2}}} \underbrace{\int_0^{\infty} y^{\frac{3}{2}} e^{-y} dy}_{\text{Gamma function}}$$

Gamma function $\Gamma(t) = \int_0^{\infty} x^{t-1} e^{-x} dx$

$$= 2 \beta C_3 \cdot \frac{1}{(\beta C_2)^{\frac{5}{2}}} \Gamma\left(\frac{5}{2}\right) = 2 \beta C_3 \cdot \frac{1}{(\beta C_2)^{\frac{5}{2}}} \cdot \frac{3}{4} \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} (1 + \beta C_4 x^4) e^{-\beta C_2 x^2} dx = 2 \int_0^{\infty} e^{-\beta C_2 x^2} dx + 2 \int_0^{\infty} \beta C_4 x^4 e^{-\beta C_2 x^2} dx$$

↑

Similar to previous one

$$= 2 \int_0^{\infty} \frac{y^{-\frac{1}{2}}}{\sqrt{\beta C_2}} e^{-y} dy + 2 \beta C_4 \cdot \frac{1}{(\beta C_2)^{\frac{5}{2}}} \cdot \frac{3}{4} \sqrt{\pi}$$

$$= \frac{2}{\sqrt{\beta C_2}} \Gamma\left(\frac{1}{2}\right) + 2 \beta C_4 \frac{1}{(\beta C_2)^{\frac{5}{2}}} \cdot \frac{3}{4} \sqrt{\pi}$$

$$= \frac{2}{\sqrt{\beta C_2}} \sqrt{\pi} + 2 \beta C_4 \frac{1}{(\beta C_2)^{\frac{5}{2}}} \cdot \frac{3}{4} \sqrt{\pi}$$

Problem 5.1)

a) Continued.

$$\begin{aligned}
 \langle x \rangle &= \frac{\cancel{\frac{2\sqrt{\pi}}{\sqrt{\beta C_2}}} \beta C_3 (\beta C_2)^{-\frac{5}{2}} \cdot \frac{3}{4} \sqrt{\pi}}{\cancel{\frac{2\sqrt{\pi}}{\sqrt{\beta C_2}}} + \cancel{\beta C_4 \cdot (\beta C_2)^{-\frac{5}{2}} \cdot \frac{3}{4} \sqrt{\pi}}} = \frac{\beta C_3 \cdot \frac{3}{4}}{(\beta C_2)^2 + \beta C_4 \cdot \frac{3}{4}} \\
 &= \frac{3 C_3 \beta}{4 \beta^2 C_2^2 + 3 \beta C_4} = \frac{3 \left(\frac{C_3}{\beta} \right)}{4 C_2^2 + 3 \left(\frac{C_4}{\beta} \right)}, \quad \beta = \frac{1}{k_B T} \\
 &= \frac{3 C_3 k_B T}{4 C_2^2 + 3 C_4 k_B T} \quad \# \quad \text{qed.}
 \end{aligned}$$

Neglect the fourth power term.

$$\langle x \rangle \approx \frac{3 C_3 k_B T}{4 C_2^2}$$

$$\text{Coefficient of thermal expansion} = \frac{\partial \langle x \rangle}{\partial T}$$

$$= \frac{3 C_3 k_B}{4 C_2^2} \quad \#$$

Problem 5.1)

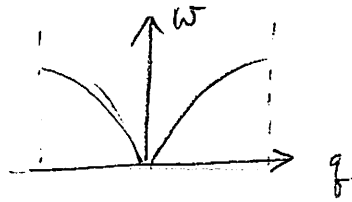
$$b) \quad \vec{J}_{\text{heat}} = \sum_{\vec{q}} N_{\vec{q}} \cdot \hbar \omega_{\vec{q}} \cdot \vec{v}_{\vec{q}} = -K_L \cdot \nabla T$$

$$\frac{N_{\vec{q}} - N_{\vec{q}}^0}{\tau_{\vec{q}}} = - (\vec{v}_{\vec{q}} \cdot \nabla T) \frac{\partial N_{\vec{q}}^0}{\partial T}$$

$$N_{\vec{q}} = N_{\vec{q}}^0 - (\vec{v}_{\vec{q}} \cdot \nabla T) \tau_{\vec{q}} \frac{\partial N_{\vec{q}}^0}{\partial T}$$

$$\sum_{\vec{q}} \left(N_{\vec{q}}^0 - (\vec{v}_{\vec{q}} \cdot \nabla T) \frac{\partial N_{\vec{q}}^0}{\partial T} \tau_{\vec{q}} \right) \hbar \omega_{\vec{q}} \vec{v}_{\vec{q}} = -K_L \cdot \nabla T$$

$$\vec{v}_{\vec{q}} = \frac{1}{\hbar} \frac{\partial \hbar \omega}{\partial \vec{q}}$$



$\vec{v}_{\vec{q}}$ is asymmetric around $\vec{q}=0$.

$$\Rightarrow \sum_{\vec{q}} N_{\vec{q}}^0 \hbar \omega_{\vec{q}} \cdot \vec{v}_{\vec{q}} = 0$$

$$\Rightarrow - \sum_{\vec{q}} (\vec{v}_{\vec{q}} \cdot \nabla T) \frac{\partial N_{\vec{q}}^0}{\partial T} \hbar \omega_{\vec{q}} \vec{v}_{\vec{q}} \tau_{\vec{q}} = -K_L \cdot \nabla T$$

$$N_{\vec{q}}^0 = \frac{1}{e^{\frac{\hbar \omega_{\vec{q}}}{k_B T}} - 1} \left(\frac{1}{V} \right) \text{ (Bose - Einstein distribution)}$$

number per unit volume

$$K_L = \sum_{\vec{q}} |\vec{v}_{\vec{q}}|^2 \hbar \omega_{\vec{q}} \cdot \frac{\hbar \omega_{\vec{q}} e^{\frac{\hbar \omega_{\vec{q}}}{k_B T}}}{k_B T^2 (e^{\frac{\hbar \omega_{\vec{q}}}{k_B T}} - 1)^2} \tau_{\vec{q}}$$

$$\sum_{\vec{q}} \rightarrow \int d\vec{q}$$

Problem 5.1)

b) Continued. Debye approximation $\Rightarrow \omega_q = q \cdot v_s$

$$D(\omega) d\omega = \frac{4\pi q^2 dq}{\left(\frac{2\pi}{L}\right)^3} = \frac{4\pi q^2 \cdot dq}{(2\pi)^3} V = \frac{\cancel{4\pi} q^2 dq V}{\cancel{8\pi} 2} = \frac{q^2 dq \cdot V}{2\pi^2}$$

$$D(\omega) = \frac{V q^2}{2\pi^2} \left(\frac{d\omega}{dq}\right)^{-1} = \frac{V q^2}{2\pi^2} \cdot \frac{1}{v_s} = \frac{V \omega^2}{2\pi^2 v_s^3}$$

$$\sum_q \rightarrow \int_0^{q_D} d^3 \vec{q} = \int_0^{\omega_D} D(\omega) d\omega$$

$$K_L = \int_0^{\omega_D} \frac{V \omega_q^2}{2\pi^2 v_s^3} \tau_q v_s^2 \cdot \hbar \omega_q \left(\frac{1}{V}\right) \frac{\hbar \omega_q e^{\frac{\hbar \omega_q}{k_B T}}}{k_B T^2 (e^{\frac{\hbar \omega_q}{k_B T}} - 1)^2} d\omega_q$$

$$= \frac{1}{2\pi^2 v_s} \int_0^{\omega_D} (\hbar \omega_q)^2 \frac{\omega_q^2 e^{\frac{\hbar \omega_q}{k_B T}}}{\tau_q^{-1} k_B T^2 (e^{\frac{\hbar \omega_q}{k_B T}} - 1)^2} d\omega_q$$

Let $\frac{\hbar \omega_q}{k_B T} = x$, $\frac{\hbar \omega_D}{k_B T} = x_D$, $\theta_D = \frac{\hbar \omega_D}{k_B} \Rightarrow x_D = \frac{\theta_D}{T}$

$$K_L = \frac{\hbar^2}{2\pi^2 v_s} \int_0^{x_D} \frac{\left(\frac{k_B T}{\hbar}\right)^4 x^4 \cdot e^x}{\tau_q^{-1} k_B T^2 (e^x - 1)^2} \cdot \left(\frac{k_B T}{\hbar}\right) dx$$

$$= \frac{\hbar^2}{2\pi^2 v_s} \left(\frac{1}{k_B T}\right) \left(\frac{k_B T}{\hbar}\right) \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{x_D} \frac{x^4 e^x}{\tau_q^{-1} (e^x - 1)^2} dx$$

$$= \frac{k_B}{2\pi^2 v_s} \left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{\tau_q^{-1} (e^x - 1)^2} dx \quad q=d.$$

Problem 5.1)

c)

$$\kappa_L = A \frac{\bar{M} \theta^3 \delta}{\gamma^2 T n^3}$$

n : number of atoms per unit cell

θ : traditional Debye temperature (determined by elastic constants or specific heat)

\bar{M} : average atomic mass

γ : Gruneisen parameter

A : a constant has γ – dependence

Assume it's under room temperature condition $T=300K$.

- For silicon (Si), $n = 2, \theta_a = 395K = \theta n^{-1/3}, \gamma = 1.06, \bar{M} = 28.08 \text{ amu}, \delta = 2.71\text{\AA}$.

The calculated thermal conductivity for Si is $\kappa_{Si} = 0.59 Wcm^{-1}K^{-1}$.

- For GaAs, $n = 2, \theta_a = 220K = \theta n^{-1/3}, \gamma = 0.75, \bar{M} = 72.32 \text{ amu}, \delta = 2.83\text{\AA}$.

The calculated thermal conductivity for GaAs is $\kappa_{GaAs} = 0.55 Wcm^{-1}K^{-1}$.

- For GaN, $n = 4, \theta_a = 390K = \theta n^{-1/3}, \gamma = 0.7, \bar{M} = 41.87 \text{ amu}, \delta = 2.25\text{\AA}$.

The calculated thermal conductivity for GaN is $\kappa_{GaN} = 2.01 Wcm^{-1}K^{-1}$.

- For AlN, $n = 4, \theta_a = 620K = \theta n^{-1/3}, \gamma = 0.7, \bar{M} = 20.49 \text{ amu}, \delta = 3.03\text{\AA}$.

The calculated thermal conductivity for AlN is $\kappa_{AlN} = 5.31 Wcm^{-1}K^{-1}$.

- For SiC, $n = 4, \theta_a = 740K = \theta n^{-1/3}, \gamma = 0.75, \bar{M} = 20.0 \text{ amu}, \delta = 2.18\text{\AA}$.

The calculated thermal conductivity for SiC is $\kappa_{SiC} = 5.61 Wcm^{-1}K^{-1}$.

- For BN, there is anisotropy in the thermal conductivities.

BN-xy, $n = 4, \theta_a = 1442K = \theta n^{-1/3}, \gamma = 0.75, \bar{M} = 12.4 \text{ amu}, \delta = 2.05\text{\AA}$.

The calculated thermal conductivity for BN-xy is $\kappa_{BN-xy} = 24.2 Wcm^{-1}K^{-1}$.

BN-z, $n = 4, \theta_a = 755K = \theta n^{-1/3}, \gamma = 2, \bar{M} = 12.4 \text{ amu}, \delta = 2.05\text{\AA}$.

The calculated thermal conductivity for BN-z is $\kappa_{BN-z} = 0.44 Wcm^{-1}K^{-1}$.

- For Diamond, $n = 2, \theta_a = 1450K = \theta n^{-1/3}, \gamma = 0.75, \bar{M} = 12.01 \text{ amu}, \delta = 1.78\text{\AA}$.

The calculated thermal conductivity for Diamond is $\kappa_{Diamond} =$

$16.42 Wcm^{-1}K^{-1}$.

Problem 5.1)

d)

Intuitively, when there is an additional scattering process, the overall thermal conductivity should decrease. It can be explained using the Part b's expression for thermal conductivity.

$$\kappa_L = \frac{k_B}{2\pi^2 v_s} \left(\frac{k_B T}{\hbar} \right)^3 \int_0^{\theta_D/T} dx \frac{x^4 e^x}{\tau_q^{-1}(x)(e^x - 1)^2}$$

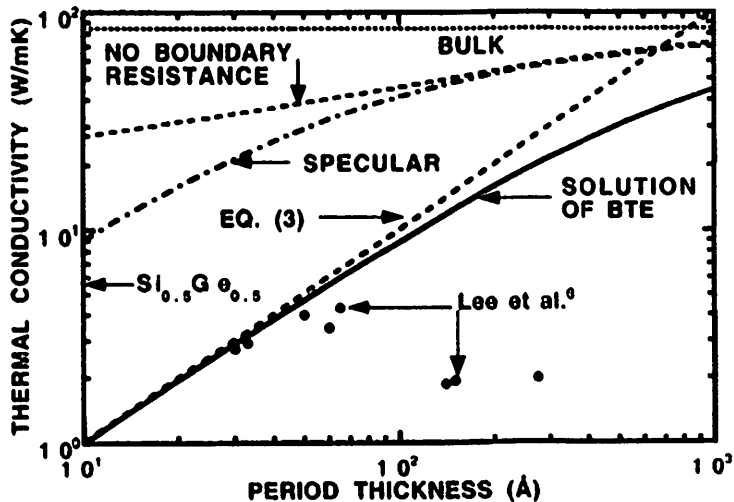
$$\kappa_L \propto \tau_q$$

And the total relaxation time can be evaluated as following.

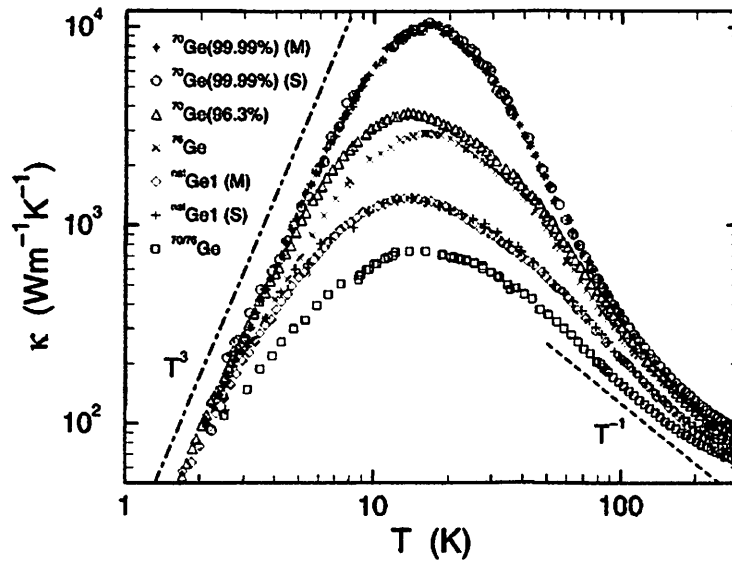
$$\tau_q^{-1} = \sum_i \tau_i^{-1}$$

If there is one more scattering term, the total relaxation time will decrease, then reduces the thermal conductivity.

- For alloys, we can expect that the relaxation time would be reduced due to the alloy scattering process.
- For superlattices, there are several scattering processes in comparison with its binary constituents. When the superlattice's thickness is below critical thickness, the reduction is due to diffuse interface scattering. G. Chen et al used Boltzmann transport equation to solve the thermal conductivity reduction behavior in the Si/Ge superlattices. [1] As show in following figure, the cross plane thermal conductivity is reduced two order compared with bulk part. When the superlattice's thickness exceeds the critical thickness, the dislocation scattering becomes the dominant scattering process.



- For isotopes, there is isotopes scattering in the crystal. As we can see from Asen-Palmer et al's article [2], the pure ^{70}Ge (99.99%) has the highest thermal conductivity. As the crystal contains more isotopes, the thermal conductivity starts decreasing due to the isotope scattering process.



[1] Chen, G. and Neagu, M., "Thermal conductivity and heat transfer in superlattices", Applied Physics Letters, 71, 2761-2763 (1997),

DOI:<http://dx.doi.org/10.1063/1.120126>

[2] M. Asen-Palmer, K. Bartkowski, E. Gmelin, M. Cardona, A. P. Zhernov, A. V.

Inyushkin, A. Taldenkov, V. I. Ozhogin, K. M. Itoh, and E. E. Haller, "Thermal conductivity of germanium crystals with different isotopic compositions", Phys. Rev. B 56, 9431

Problem 5.2)

a) Rockett Problem 10.14. # 1.

(a) Distance between substrate and source = 30 cm

$$3\lambda_{mfp} = 30 \text{ cm}$$

$$\Rightarrow \lambda_{mfp} = 10 \text{ cm}$$

$$\sigma = 4 \times 10^{-15} \text{ cm}^2$$

Equation 10.1

$$\lambda_{mfp} = \frac{k_B T}{\sqrt{2} \sigma P}, \quad T = 300 \text{ K}$$

$$P = \frac{k_B T}{\sqrt{2} \sigma \cdot \lambda_{mfp}} = 7.32 \times 10^{-2} \text{ Pa} = 5.49 \times 10^{-4} \text{ Torr}$$

#

(b) $T = 1000 \text{ K}$

$$P = 2.44 \times 10^{-1} \text{ Pa} = 1.83 \times 10^{-3} \text{ Torr}$$

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Problem 5.2)

b) Rockett. Problem 10.14 #2.

(a)

$$F = \frac{P}{\sqrt{2\pi m k_B T}}$$

$$F_{Ga} = 5 \times 10^{14} \text{ cm}^{-2} \cdot \text{s}^{-1} = \frac{P_{Ga}}{\sqrt{2\pi m_{Ga} k_B T_{Ga}}}$$

$$P_{Ga} = 5 \times 10^{-4} \text{ Pa}$$

$$F_{As_4} = 2 \times 10^{16} \text{ cm}^{-2} \cdot \text{s}^{-1} = \frac{P_{As_4}}{\sqrt{2\pi m_{As_4} k_B T_{As_4}}}$$

$$P_{As_4} = 2.94 \times 10^{-2} \text{ Pa}$$

(b)

$$\sigma = 4 \times 10^{-15} \text{ cm}^2 = 4 \times 10^{-19} \text{ m}^2$$

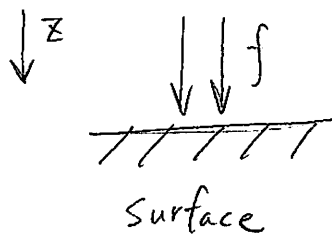
$$\lambda_{mfp, Ga} = \frac{k_B T_{Ga}}{\sqrt{2} \sigma P_{As_4}} = 0.83 \text{ m} = 83 \text{ cm}$$

(c)

No, the Ga atom wouldn't be scattered significantly by As_4 vapors. The mean free path for Ga atom in As_4 vapor is almost one meter long. A typical MBE or other growth chamber's substrate to source distance is smaller than this value. Therefore, there would be very small chance for Ga atom to be scattered by As_4 atom.

Problem 5.3)

a)



Assume the gas particle's velocity distribution is Maxwell-Boltzmann distribution.

$$P(v_x, v_y, v_z) = C \cdot e^{-\frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) / k_B T}$$

\uparrow
 normalization constant

$$1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dv_x dv_y dv_z C \cdot e^{-\frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) / k_B T}$$

$$= C \cdot \left(\sqrt{\frac{\pi}{\frac{m}{2k_B T}}} \right)^3 = C \cdot \frac{(2k_B T \pi)^{\frac{3}{2}}}{m^{\frac{3}{2}}}$$

$$C = \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}}$$

We're considering only those particles hitting surface. (Negative v_z won't hit)

$$f = C \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_0^{\infty} dv_z \cdot v_z \cdot n \cdot e^{-\frac{m}{2k_B T} (v_x^2 + v_y^2 + v_z^2)}$$

\uparrow
 Particle density

$$= \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} \cdot \frac{2\pi k_B T}{m} \cdot n \int_0^{\infty} dv_z \cdot v_z \cdot e^{-\frac{m}{2k_B T} v_z^2}$$

$$= \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} \left(\frac{2\pi k_B T}{m} \right) \cdot n \cdot \frac{1}{\cancel{\left(\frac{m}{2k_B T} \right)}} = \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} \frac{2\pi n k_B T}{m^2} \cdot k_B T$$

Note: $pV = Nk_B T \Rightarrow p = n k_B T$

$$= \left(\frac{1}{2\pi k_B T} \right)^{\frac{3}{2}} \cdot \frac{2\pi}{m^{\frac{1}{2}}} \cdot p \cdot k_B T = \frac{p}{\sqrt{2\pi m k_B T}} \quad \# \text{ ged.}$$

Problem 5.3)

b)

$$P_1 \approx 10^{-10} \text{ Torr} = 133 \times 10^{-10} \text{ Pa} = 1.33 \times 10^{-8} \text{ Pa}$$

$$f = \frac{P}{\sqrt{2\pi m k_B T}} = \frac{1.33 \times 10^{-8}}{\sqrt{2\pi m k_B T}}$$

$$m = 14 \times 2 \text{ amu} = 28 \text{ amu} = 28 \times 1.66 \times 10^{-27} \text{ kg}$$

$$f = 3.82 \times 10^{14} \text{ molecules/m}^2 \cdot \text{s}$$

$$= 3.82 \times 10^{14} \text{ molecules} / (100)^2 \text{ cm}^2 \cdot \text{s}$$

$$= 3.82 \times 10^{10} \text{ molecules/cm}^2 \cdot \text{s}$$

#

No, I don't think there would be growth on the GaN surface.

N₂ molecules can be adsorbed on the GaN surface.

But the bonding between nitrogen atoms are very strong, and can't be broken easily. Generally, it would require a plasma source to break the bonding of N₂ molecules.

Problem 5.3)

c)

$$P_1 \approx 10^{-10}$$

$$P_1 V = N_1 k_B T$$

$$N_1 = \frac{P_1 V}{k_B T}$$

$$P_2 V = (N_1 + N_2) k_B T = \left(\frac{P_1 V}{k_B T} + N_2 \right) k_B T$$

$$P_2 \approx 10^{-9}$$

$$= P_1 V + N_2 k_B T$$

$$N_2 k_B T = (P_2 - P_1) V$$

$$f_0 = \frac{P_2 - P_1}{\sqrt{2\pi m k_B T}} = \frac{(10^{-9} - 10^{-10}) \times 133}{\sqrt{2\pi m_0 k_B T}} = 4.55 \times 10^{15} \text{ atoms/m}^2 \cdot \text{s}$$

$$m_0 = 16 \text{ amu}$$

$$f_0 = 4.55 \times 10^{11} \text{ atoms/cm}^2 \cdot \text{s}$$

Sticking coefficient

$$O \text{ Atoms incorporated into GaN surface} = f_0 \cdot S$$

$$= 4.55 \times 10^{11} \times 0.05 = 2.28 \times 10^{10} \text{ atoms/cm}^2 \cdot \text{s}$$

Leak was instantaneous. And GaN exposed to Oxygen for 10 min.

$$O \text{ Atoms onto GaN Surface} = 600 \text{ s} \times 2.28 \times 10^{10} \text{ atoms/cm}^2 \cdot \text{s}$$

$$= 1.37 \times 10^{13} \text{ atoms/cm}^2$$

#

Problem 5.3)

d)

The contamination oxygen incorporated into the surface will cause additional doping to GaN. Therefore, it induces band bending at the interface. This band bending then becomes the barrier for hole transport.

This is the simulation result from 1D Poisson. I assume the interface thickness is 1nm.

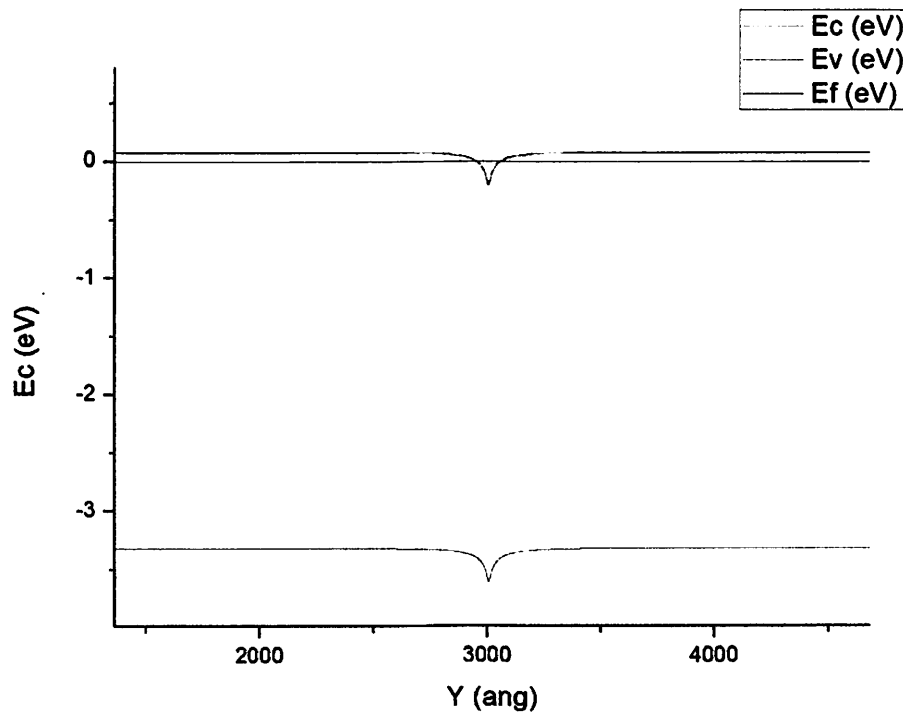
The total sheet impurity concentration should be the same, which means

$$\sigma_o = 1.37 \times 10^{13} \text{ cm}^{-2}$$

Effective donor concentration is

$$N_D = \frac{\sigma_o}{1 \times 10^{-7} \text{ cm}} = 1.37 \times 10^{20} \text{ cm}^{-3}$$

We can estimate the barrier height for hole transport using 1D Poisson.



The barrier height is estimated to be 0.286eV.

Problem 5.4)

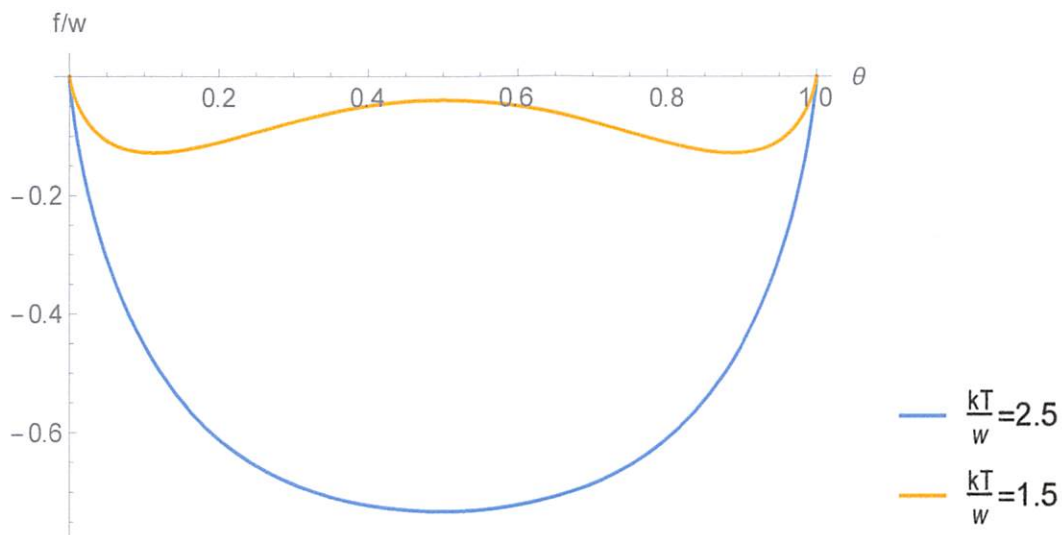
a)

From Taso's Chapter 6, we can write down the free energy per site as following.

$$\frac{f_{adat}}{\omega} = 4\theta(1 - \theta) + \frac{kT}{\omega} [\theta \ln \theta + (1 - \theta) \ln(1 - \theta)]$$

With the above equation, we can draw the plot for two normalized temperatures.

The orange curve represents a low temperature case, and the surface is in phase separated. The blue curve represents a high temperature, and the surface is in rough phase.

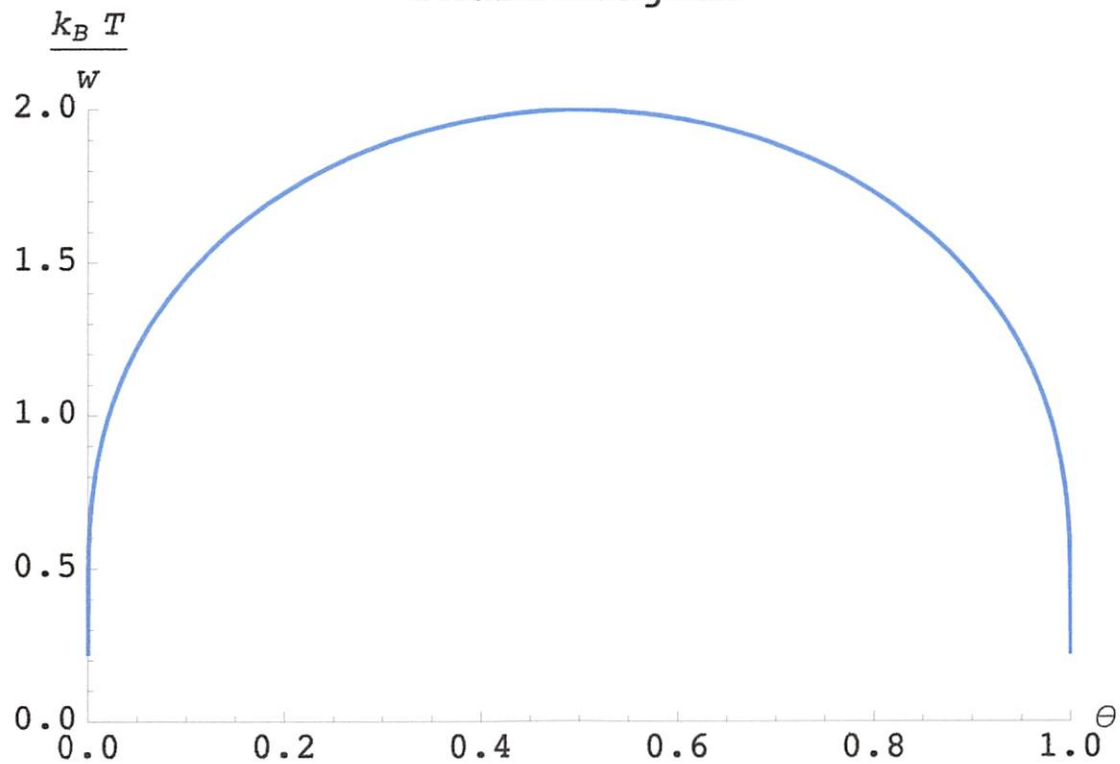


We can also plot the phase diagram. The phase diagram represents the minimum free energy situations. We can just take the first derivative of the above equation to find the extremum of free energy.

$$\frac{\partial}{\partial \theta} \left(\frac{f_{adat}}{\omega} \right) = 0$$

$$\frac{kT}{\omega} = \frac{-4(1-\theta) + 4\theta}{-\ln(1-\theta) + \ln\theta}$$

Phase Diagram



Problem 5.4)

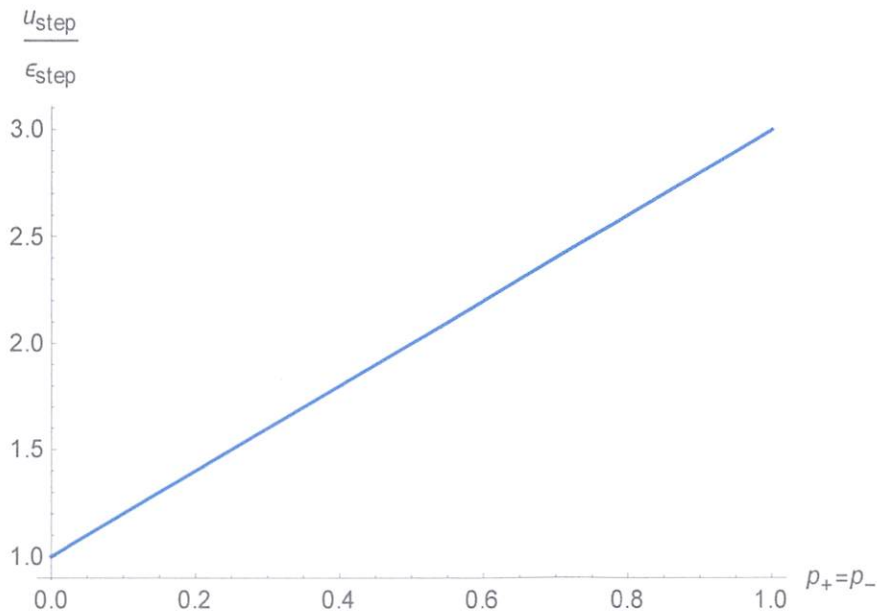
b)

From Eq. 6.13 in Taso's book, we can write down the free energy and entropy of step.

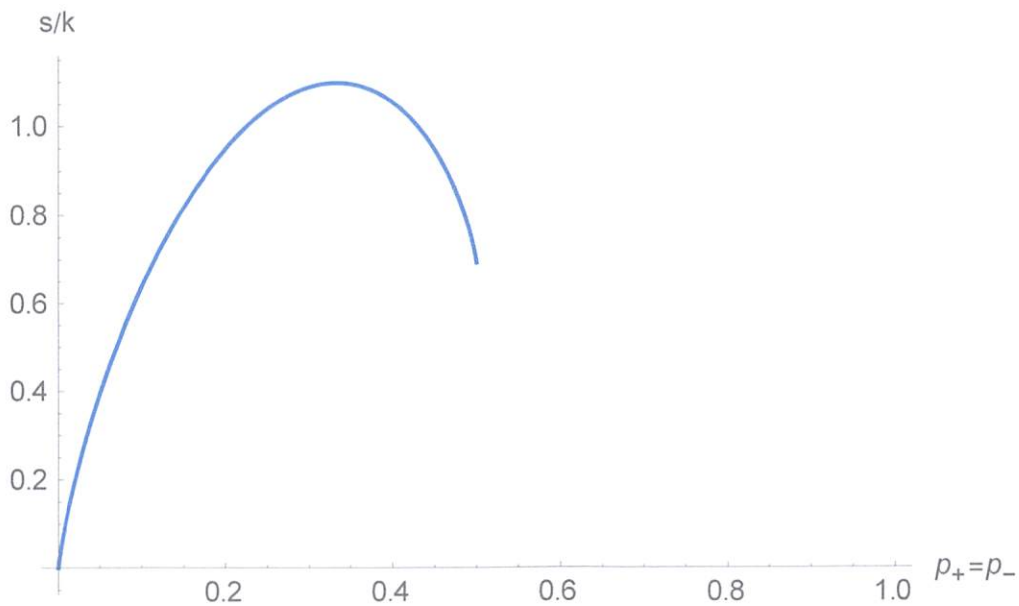
$$u_{step} = \epsilon_{step} + 2\epsilon_{kink}p_-$$

$$-\frac{s_{step}}{k} = 2p_- \ln(p_-) + (1 - 2p_-) \ln(1 - 2p_-)$$

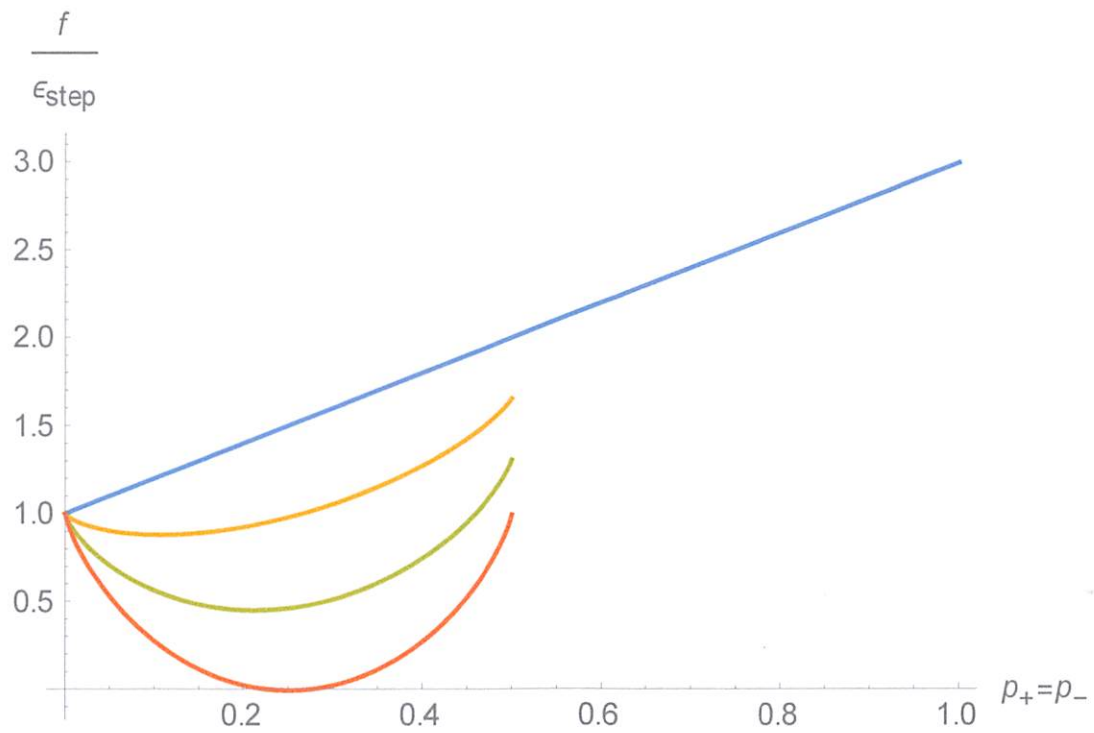
$$f_{step} = u_{step} - Ts_{step}$$



Step energy v.s probability of having kinks.



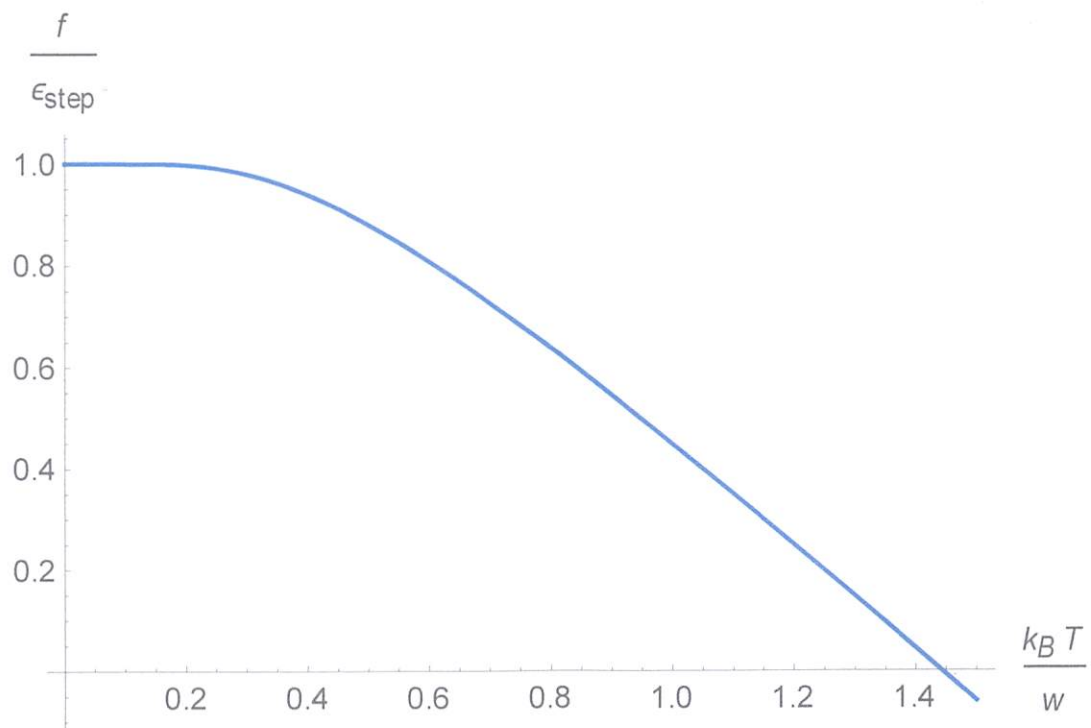
Entropy v.s probability of having kinks.



Free energy v.s probability of having kinks. Blue corresponds to zero

temperature. Orange corresponds to $\frac{kT}{\omega} = 0.5$. Green corresponds to $\frac{kT}{\omega} = 1$.

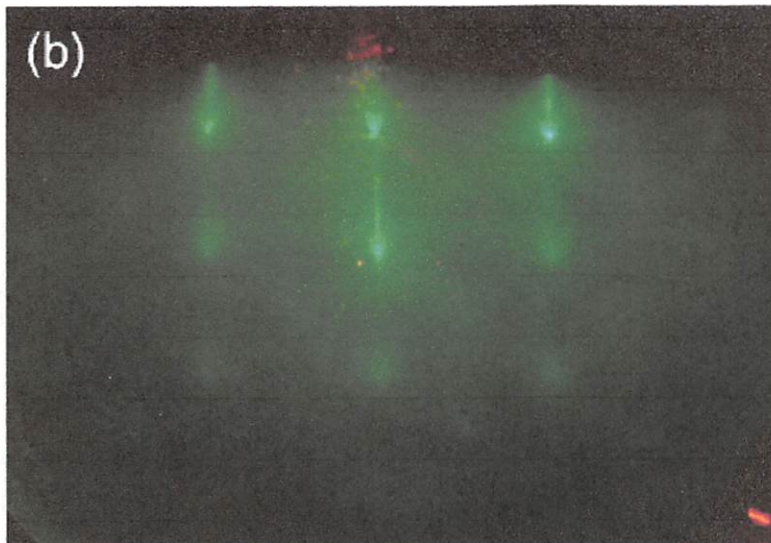
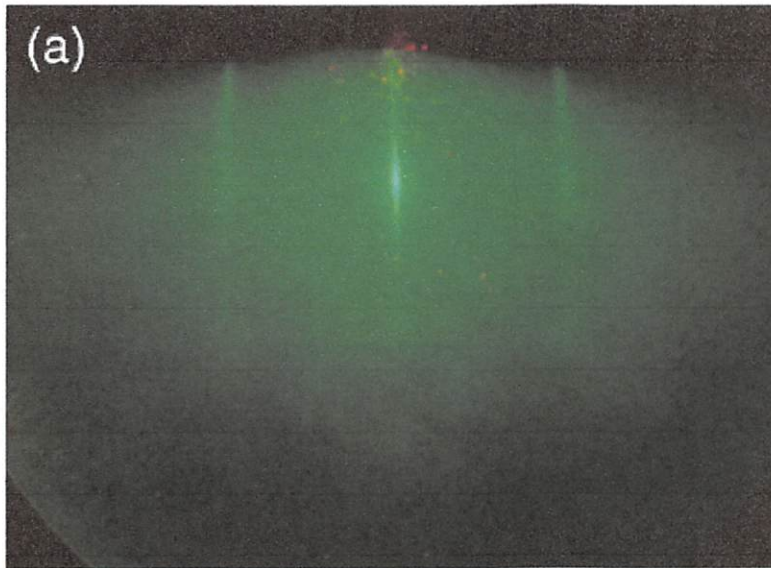
Red corresponds to $\frac{kT}{\omega} = 1.45$.



Problem 5.4)

c)

For the first surface roughing or phase separated case, it is very common in MBE system to use RHEED to observe these phenomenon. By the RHEED patterns, we can tell whether the growing surface is in layer by layer mode or island mode. We can change substrate temperature or source beam flux to drive the sample's surface states into different regimes in the phase diagram.



(a) RHEED pattern of smooth GaN surface.

(b) RHEED pattern of rough GaN surface.

If we want to do in-situ measurement on the surface behavior, RHEED probably is the best choice. For post-characterization, AFM or STM might be another choice to exactly determine the surface state through scanning image.

5.1) a. Given the potential energy $U(x) = c_2 x^2 - c_3 x^3 - c_4 x^4$, the thermal average from Boltzmann statistics is $\langle x \rangle = \frac{\int_{-\infty}^{\infty} dx x e^{-\beta U}}{Z} = \frac{\int_{-\infty}^{\infty} dx x e^{-\beta U}}{\int_{-\infty}^{\infty} dx e^{-\beta U}}$. For small anharmonicity:

$e^{-\beta U} \approx e^{-\beta c_2 x^2} (1 + c_3 x^3 + c_4 x^4)$, so:

- $\int_{-\infty}^{\infty} dx x e^{-\beta U} = \int_{-\infty}^{\infty} dx e^{-\beta c_2 x^2} (x + c_3 x^4 + c_4 x^5)$. x and x^5 are odd, $e^{-\beta c_2 x^2}$ is even, so they integrate to 0. $\Rightarrow \langle x \rangle = \int_{-\infty}^{\infty} dx c_3 x^4 e^{-\beta c_2 x^2} = \frac{3}{4} \frac{c_3 \sqrt{\pi}}{c_2^{5/2} \beta^{3/2}}$
- $\int_{-\infty}^{\infty} dx e^{-\beta U} = \int_{-\infty}^{\infty} dx e^{-\beta c_2 x^2} (1 + c_3 x^3 + c_4 x^4) = \frac{\sqrt{\pi}}{4 c_2^{5/2}} \left(\frac{3 c_4}{\beta^{3/2}} + \frac{4 c_3^2}{\beta^{5/2}} \right)$

so in total $\langle x \rangle = \frac{3 c_3}{c_2^{5/2} \beta^{3/2}} \left(\frac{\beta^{3/2}}{3 c_4 + 4 c_3^2 \beta} \right) = \boxed{\frac{3 c_3 K T}{4 c_2^2 + 3 c_4 K T}}$, with $\beta = \frac{1}{K T}$ as usual.

Neglecting c_4 , $\frac{\partial \langle x \rangle}{\partial T} = \frac{\partial}{\partial T} \frac{3 c_3 K T}{4 c_2^2} = \boxed{\frac{3 c_3 K}{4 c_2^2}}$

b. Starting with $J_{\text{heat}} = \sum_q N_q \hbar \omega_q v_q$, we need N_q :

$\frac{N_q - N_q^0}{\tau_q} = -(\vec{v}_q \cdot \vec{\nabla}_T) \frac{\partial N_q^0}{\partial T}$ in the steady state ($\frac{\partial N_q}{\partial t} = 0$)

$\Rightarrow N_q = N_q^0 - \tau_q v_q \nabla T \frac{\partial N_q^0}{\partial T}$, where the vectors have been dropped.

Right away we can see the first term will integrate to 0, because $N_q^0 \omega_q = N_{-q}^0 \omega_{-q}$ and $v_q = -v_{-q}$, so $\sum_{q=-\infty}^{\infty} N_q \omega_q \hbar v_q = - \sum_{q=0}^{\infty} N_q \hbar \omega_q v_q$ so the sum = 0.

Now ω and q are continuous, so we need to convert the sum into an integral:

$J_{\text{heat}} = \int_0^{\omega_{\text{max}}} N_q \hbar \omega_q v_q g(q) dq$, where the density of states has been used, and now the integration is w.r.t ω instead of q .

$N_q^0 = \frac{1}{e^{\hbar \omega / K T} - 1}$ by Bose-Einstein stat., so $\frac{\partial N_q^0}{\partial T} = \frac{-1}{(e^{\hbar \omega / K T} - 1)^2} e^{\hbar \omega / K T} \frac{\hbar \omega}{K} \left(\frac{-1}{T^2} \right)$

$\Rightarrow J_{\text{heat}} = \int_0^{\omega_{\text{max}}} -\tau_q v_q \nabla T \frac{\hbar \omega}{K T^2} \frac{e^{\hbar \omega / K T}}{(e^{\hbar \omega / K T} - 1)^2} \hbar \omega v_q g(\omega) d\omega$.

$J_{\text{heat}} = -k_L \nabla T$, and also $g(q) = \frac{q^2}{2\pi^2 v_s}$, assuming linear dispersion $v_q = v_s = \text{speed of sound}$

and $\omega = q v$, so $g(\omega) = \frac{\omega^2}{2\pi^2 v_s^3}$. All together, then

$-k_L \nabla T = \int_0^{\omega_{\text{max}}} -\tau_L v_s^2 \nabla T \frac{\hbar^2 \omega^2}{K T^2} \frac{\omega^2}{2\pi^2 v_s^3} \frac{e^{\hbar \omega / K T}}{(e^{\hbar \omega / K T} - 1)^2} d\omega$

or $K_L = \frac{\hbar^2}{KT^2} \frac{1}{2\pi^3 V_s} \int_0^{\omega_{\max}} \tau_2 \omega^4 \frac{e^{\hbar\omega/KT}}{(e^{\hbar\omega/KT} - 1)^2} d\omega$. Making the sub. $x = \frac{\hbar\omega}{KT}$, $dx = \frac{\hbar}{KT} d\omega$:

$\Rightarrow K_L = \frac{\hbar^2}{KT^2} \frac{1}{2\pi^3 V_s} \left(\frac{KT}{\hbar} \right)^4 \int_0^{x_{\max}} \tau_2 x^4 \frac{e^x}{(e^x - 1)^2} dx$. Finally $x_{\max} = \frac{\hbar\omega_{\max}}{KT} = \frac{\Theta_D}{T}$ by definition

So $K_L = \frac{K}{2\pi^3 V_s} \left(\frac{KT}{\hbar} \right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x}{\tau_2 (e^x - 1)^2} dx$

- c. $K_L = A \frac{\bar{M} \Theta_D^3}{T^2 n^{2/3}}$
- A is a "constant" that depends weakly on γ
 - \bar{M} is the average mass of the unit cell containing n atoms
 - Θ is the "traditional" Debye temperature, determined from specific heat, that takes into account all available modes, not just acoustic.
 - δ^3 is the volume per atom
 - γ is the Grüneisen parameter, which characterizes the anharmonicity of the material defined by $\gamma = -\frac{d \ln \omega_i}{d \ln V}$
 - T is the temperature
 - n is the # of atoms in the unit cell

At 300 K, the values I get are

Si: $0.59 \text{ W cm}^{-1} \text{ K}^{-1}$	GeAs: $0.55 \text{ W cm}^{-1} \text{ K}^{-1}$	GaN: $2.01 \text{ W cm}^{-1} \text{ K}^{-1}$
AlN: $3.82 \text{ W cm}^{-1} \text{ K}^{-1}$	SiC: $5.61 \text{ W cm}^{-1} \text{ K}^{-1}$	BN: $11.05 \text{ W cm}^{-1} \text{ K}^{-1}$
Diamond: $16.42 \text{ W cm}^{-1} \text{ K}^{-1}$		

Using the parameters in the article, and $\Theta_a = \Theta n^{-1/3} \Rightarrow K = A \frac{\bar{M} \Theta_a^3 \delta n^{1/3}}{T^2}$

Some of these are slightly different from what they report, but in theory we should be using the same equation...

d. Compound semiconductor alloys and superlattices are made up of different types of atoms, so phonon scattering is greatly increased and the thermal conductivity decreases. Each different atom effectively acts like an impurity with a different mass, and the mass contrast causes the K_L contrast.

In the same way, isotopes have a different mass than the normal atoms and also scatter phonons and therefore also decrease the thermal conductivity. Again the different isotopes act like impurities.

Generally electronic devices like transistors need a high thermal conductivity because the heating due to transistor density is currently one of the biggest factors preventing ICs from being faster than $\sim 3 \text{ GHz}$. Lasers and LEDs also require a high K_L to dissipate heat from non-radiative relaxations.

d. (cont.) Low thermal conductivity is needed in materials with a strong thermoelectric effect. If the electrical conductivity is high and the thermal conductivity is low, a temperature difference can induce a voltage difference / current. If the thermal conductivity is too high, the temperature difference will just dissipate right away.

5.2) 1. a. The question says you want "at least 3 mean-free-path lengths" from the source to the substrate, but I'm assuming they mean you want the path from source to substrate to be $1/3$ of the mean free path to avoid significant scattering:

$$\left. \begin{array}{l} \lambda = 90 \text{ cm} \\ \sigma = 4 \times 10^{-15} \text{ cm}^2 \\ T = 300 \text{ K} \end{array} \right\} \text{ From } \lambda = \frac{kT}{\sqrt{2}\sigma P} \Rightarrow P = \frac{kT}{\sqrt{2}\sigma\lambda} = \boxed{8 \times 10^{-3} \text{ Pa}}$$

b. Now with $T = 1000 \text{ K}$, $P = \frac{kT}{\sqrt{2}\sigma\lambda} = \boxed{2.7 \times 10^{-2} \text{ Pa}}$

2. a. The flux is related to the pressure by

$$F = 2.63 \times 10^{17} \frac{P}{\sqrt{mT}} \text{ cm}^{-2} \text{ s}^{-1}, \text{ so } P = \frac{F \sqrt{mT}}{2.63 \times 10^{17}} \text{ Pa, if } F \text{ is in cm}^{-2} \text{ s}^{-1}, m \text{ is in amu, } T \text{ in K}$$

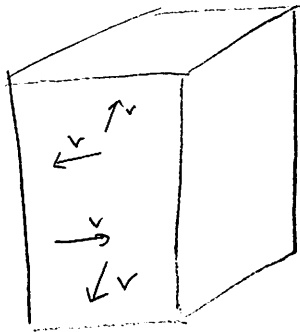
$$\Rightarrow \boxed{P_{\text{Ga}} = 0.502 \text{ Pa}, P_{\text{As}_4} = 29.45 \text{ Pa}}$$

b. $\lambda = \frac{kT}{\sqrt{2}\sigma P}$, so using T_{Ga} and P_{Ga} with $\sigma = 4 \times 10^{-15} \text{ cm}^2$

$$\boxed{\lambda = 0.828 \text{ mm}}$$

c. If the assumption that As_4 is really prevalent from the source to the substrate in the same path as the Ga is valid, then the As_4 would scatter the Ga significantly because the distance between source and substrate is $\gg 1 \text{ mm}$. On the other hand, in reality the beams may not overlap the whole way, and also the atoms are moving mostly in the same direction, so in reality the scattering would happen less frequently.

5.3) a. Given an ideal gas in a container.



The gas is moving at an average speed v . Given the Maxwell-Boltzmann distribution:

$$dn = \frac{2N}{\sqrt{\pi}} \left(\frac{m}{2KT} \right)^{3/2} v^2 e^{-mv^2/2KT}, \text{ so the average speed}$$

$$\bar{v} = \int_0^\infty v dn = \sqrt{\frac{8KT}{\pi m}}$$

The gas also has some pressure P : $PV = NKT \Rightarrow \frac{N}{V} = n = \text{concentration} = \frac{P}{KT}$

Finally, the flux on 1 flat surface is $\frac{n\bar{v}}{2} \cdot \frac{1}{2}$, where 1 factor of $\frac{1}{2}$ comes from the fact that half the particles are travelling in the right direction (at the surface) and half are travelling in the wrong direction. The other $\frac{1}{2}$ comes from the fact that some of the particles are not hitting the surface directly, so the net result is a reduction of $\frac{1}{4}$.

$$\text{So: } F = \frac{n\bar{v}}{4} = \frac{P}{KT} \frac{1}{4} \sqrt{\frac{8KT}{\pi m}} = \boxed{\frac{P}{2\pi m KT}}$$

b. At $P_1 = 10^{-10}$ torr, and $m(N_2) = 28 \text{ amu} = 4.65 \times 10^{-26} \text{ kg}$
 $= 1.33 \times 10^{-8} \text{ Pa}$

$$F = \frac{P}{2\pi m KT} = \boxed{3.82 \times 10^{14} \text{ m}^{-2} \text{ s}^{-1}}$$

For a typical atom density of $5 \times 10^{14} \text{ cm}^{-2}$,

each growth site (lattice point) gets hit with $\frac{F}{n} = 7.6 \times 10^{-5} \text{ atoms/sec}$
 $= 0.28 \text{ atoms/hour}$. So on average each site is hit ~ once every 4 hours, but then it has to stick and the sticking parameter is usually very low so to a very good approximation no growth will occur.

c. In this case, $P_2 \approx P(O_2)$ because there was basically no gas in the chamber before.

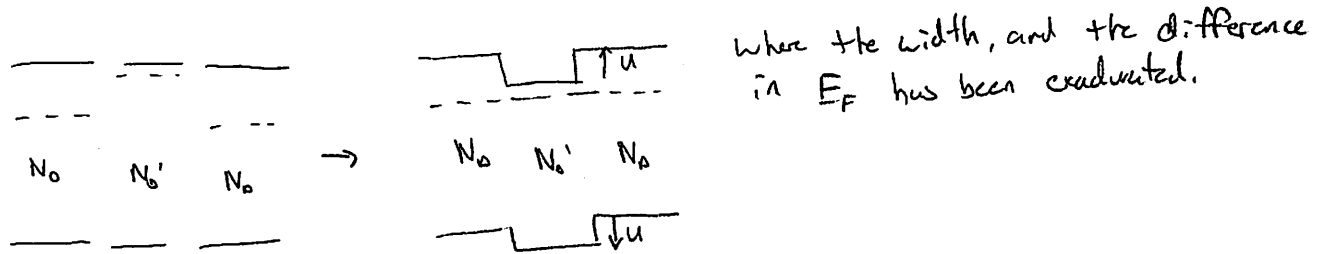
At this pressure, and with $m(O) = 16 \text{ amu} = 2.66 \times 10^{-26} \text{ kg}$

$$F = \frac{P}{2\pi m KT} = 5.05 \times 10^{15} \text{ m}^{-2} \text{ s}^{-1}. \text{ For GaN, } n = 8.9 \times 10^{22} \text{ cm}^{-3}$$

so # of atoms per area = $n^{2/3} = 2 \times 10^{19} \text{ cm}^{-2} = 2 \times 10^{19} \text{ m}^{-2}$ and the rate of replacement is $\frac{F}{\# \text{ per area}} \cdot s = 1.26 \times 10^{-5} \text{ atoms/sec}$, or in 10 min $\Rightarrow 0.00758 \text{ atoms}$

This gives an area density of oxygen of $1.52 \times 10^{17} \text{ m}^{-2} = \boxed{1.52 \times 10^{13} \text{ cm}^{-2}}$

d. The reacting material will have a small "layer" doped with Oxygen, with doping density $N_D' = (1.52 \times 10^{13} \text{ cm}^{-2})^{3/2} = 5.93 \times 10^{19} \text{ cm}^{-3}$, so the band diagram will look like:



Initially the Fermi level was at $E_F - E_c = kT \ln \frac{N_D}{N_{CB}}$, and in the O-doped region $E_F' - E_c = kT \ln \frac{N_D'}{N_{CB}}$, assuming $N_D'^+ = N_D'$, i.e. full ionization, and also making the approximation that the total doping is N_D' from the oxygen, because $N_D' \gg N_D$.

So $U = E_F' - E_F = E_c + kT \ln \frac{N_D'}{N_{CB}} - E_c - kT \ln \frac{N_D}{N_{CB}} = kT \ln \frac{N_D'}{N_D} = \boxed{165 \text{ mV}}$
is the barrier height for holes.

5.4)

a. For a surface with surface coverage θ , and atoms that make bonds with energy w , the energy of a single adatom is $4w$ b/c it is missing 4 bonds. The probability that 4 of the neighbors are also adatoms is θ each, though, so each adatom actually has an energy of $4w - 4w\theta = 4w(1-\theta)$. Finally, the probability of an adatom existing is θ , so the average energy per site is $4w\theta(1-\theta)$.

The mixing entropy comes from the mixing of adatom sites and vacancies,

so $S = -k(\theta \ln \theta + (1-\theta) \ln(1-\theta))$.

In total, normalized by the bond energy,

$$\boxed{\frac{f}{w} = 4\theta(1-\theta) + \frac{kT}{w} [\theta \ln \theta + (1-\theta) \ln(1-\theta)]}$$

This is plotted above and below the phase diagram in Figure 6.2, for $kT/w = 2.5$ and 1.5 . In the middle is the phase diagram obtained by minimizing f/w at different kT/w values.

b. In general, for steps and kinks, the energy of formation is

$U_{\text{step}} = \epsilon_{\text{kink}} (P_+ + P_-) + \epsilon_{\text{step}}$, where ϵ_{step} is the energy scale of forming a step and ϵ_{kink} is the energy scale of forming either a + kink or a - kink, and P_+ and P_- are the probabilities of forming a + kink or a - kink.

In this case we are looking at $P_+ = P_-$, i.e. the step is straight, so

$$U_{\text{step}} = 2\epsilon_{\text{kink}} P_- + \epsilon_{\text{step}}. \text{ We also assume } \epsilon_{\text{kink}} = \epsilon_{\text{step}}, \text{ so } \frac{U_{\text{step}}}{\epsilon_{\text{step}}} = 1 + 2P_-.$$

Again the same entropy of mixing is used, but this time with the 3 possibilities,

$P_+ = + \text{kink}$, $P_- = - \text{kink}$, $P_0 = \text{no kink}$, so

$$S_{\text{step}} = -K (P_+ \ln P_+ + P_- \ln P_- + P_0 \ln P_0), \text{ and with our assumptions}$$

$$P_+ = P_- \text{ and } 2P_- + P_0 = 1 \Rightarrow P_0 = 1 - 2P_-$$

$$S_{\text{step}} = -2K P_- \ln P_- - (1 - 2P_-) \ln (1 - 2P_-)$$

So in total,
$$\frac{f_{\text{step}}}{\epsilon_{\text{step}}} = 1 + 2P_- + \frac{KT}{\epsilon_{\text{step}}} [2P_- \ln P_- + (1 - 2P_-) \ln (1 - 2P_-)]$$

The normalized U_{step} , S_{step} , and f_{step} are shown in Figure 6.6, on the left.

In particular, f_{step} is shown at $\frac{KT}{\epsilon_{\text{step}}} = 0, 0.5, 1.0, \text{ and } 1.45$. The equilibrium free energies at a given $\frac{KT}{\epsilon_{\text{step}}}$ are also shown on the right. These are calculated by

minimizing $\frac{f_{\text{step}}}{\epsilon_{\text{step}}}$, and plotting the minimum $f_{\text{step}}/\epsilon_{\text{step}}$.

c. Both of these effects, considering adatom excitations and extended step excitations result in a roughening of the surface at a high enough temperature. In the case of adatoms, this is seen from the phase transition between phase-separated and smooth. In the case of steps, this is seen as $f/\epsilon_{\text{step}} < 0$ after a critical temperature which implies that steps form spontaneously. From the calculations, the critical temperature for steps is lower than that for adatoms, so physically I would expect a real system to first develop isolated steps, and then become totally rough as temperature is increased. One way to probe this in the MBE chamber is to use RHEED while changing the surface temperature. This would be done while growth is stopped, as both these effects happen as a result of temperature changes and not because of growth. So I would first grow a material, using RHEED first to tell when the coverage is about $0.8^{(10)}$ by tracking the oscillations of the intensity. At this point there should almost be a complete monolayer that is phase separated, so the intensity of the diffraction spots should be high. I would then increase the temperature without any particle flux, and track the RHEED pattern

and intensity. I would expect there to be 2 clear regions: at some T_c calculated from the step analysis the intensity would decrease slightly as steps begin to form spontaneously. Then at some higher T_c , adatoms and vacancies would become favorable and the AFED intensity would decrease even further. For this to be observed, the T_c for adatoms must be below the melting point of the material.

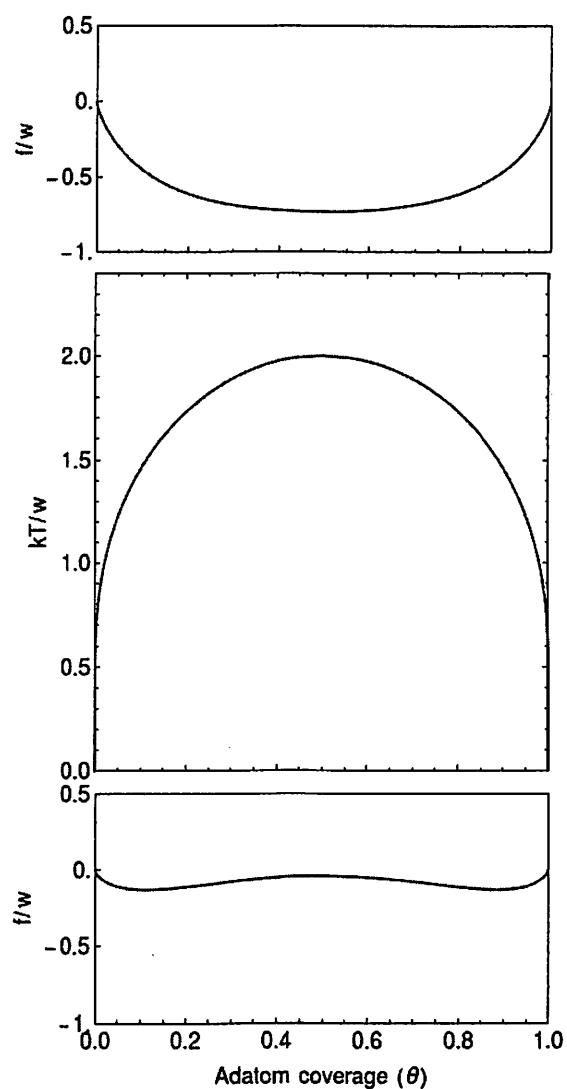


Figure 6.2: Phase diagram for surface roughening. Top and bottom show the normalized free energy at $kT/w = 2.5$ and $kT/2 = 1.5$, respectively. Middle shows the phase diagram, where below the line the surface is phase separated and above the line the surface is rough.

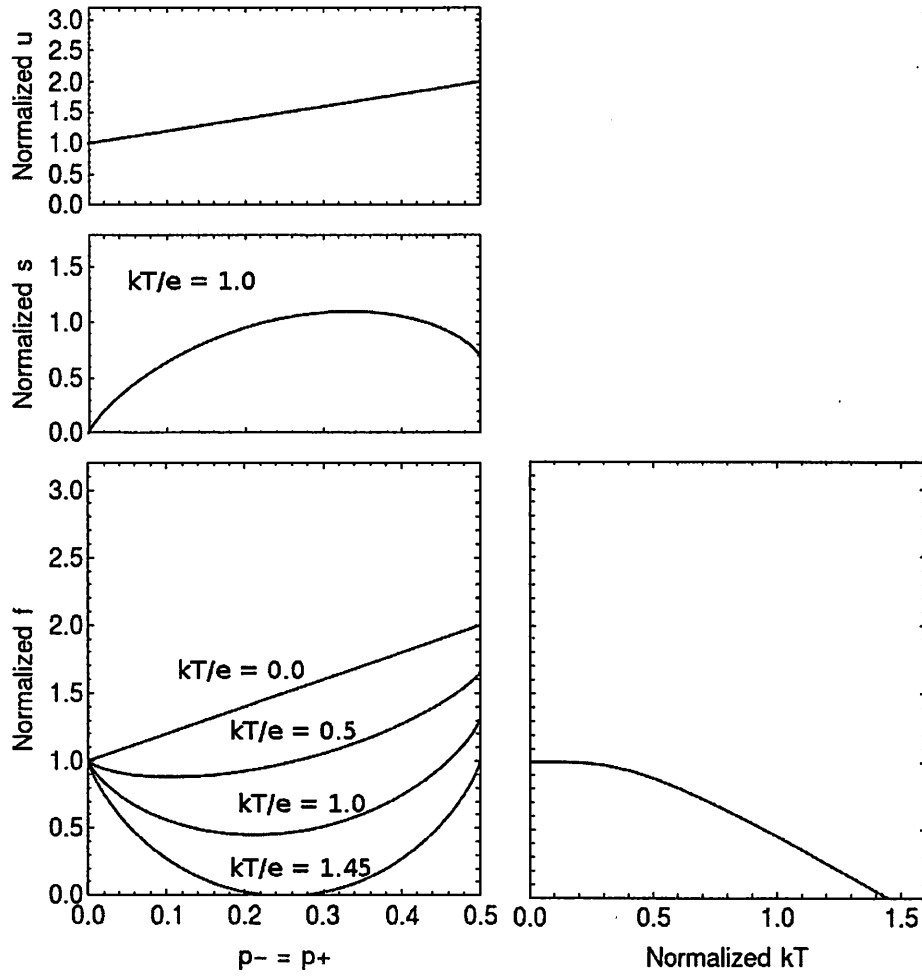


Figure 6.6: Normalized enthalpy (top), entropy (middle), and free energy (bottom) as a function of kink probability, for the case of a perfectly cut step, $\tan\phi = 0$, and kink enthalpy equal to half of the step enthalpy. Also shown on the right is the free energy minimum as a function of kT /step enthalpy.