Homework Week 3: Nanoscale and macroscale characterization
Thermoelectricity: From Atoms to Systems

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nanoHUB-U Fall 2013

Answer the **thirteen questions** including all the sub-questions below by choosing **one, best answer**. This homework does not count toward the final score, but solving and understanding this homework will be very helpful for passing the exam.

1. (Transient Harman method) when an electric current I is injected into a thermoelectric device under adiabatic conditions as shown in the figure on the right, there is heat balance at each junction between the Peltier cooling/heating, the Joule heating, and the heat conduction. For example, at the cold side at temperature T_C, the heat balance is described as

$$ST_C I - \tfrac{1}{2} I^2 R - K\Delta T = 0\,, \tag{1}$$

where S, R, K are the Seebeck coefficient, the electrical resistance, and the thermal conductance of the TE material, respectively, and $\Delta T = T_H - T_C$. Thus, a temperature gradient is created across the device, and from (1), ΔT is given by

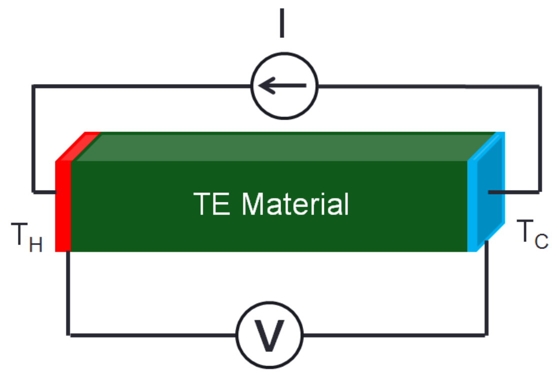
$$\Delta T = \frac{ST_C I}{K} - \frac{I^2 R}{2K}\,. \tag{2}$$

The total measured voltage across the device is comprised of the ohmic voltage plus the Seebeck voltage induced by the temperature gradient as

$$V_T = V_R + V_S = IR + S\Delta T, \tag{3}$$

where V_S is divided into the two terms, the Peltier effect-induced Seebeck voltage V_{SP} and the Joule effect-induced Seebeck voltage V_{SJ}, as

$$V_S = S\Delta T = \frac{S^2 T_C I}{K} - \frac{SI^2 R}{2K} = V_{SP} - V_{SJ}\,. \tag{4}$$



1-1. How can the figure of merit of the material, $ZT=S^2T_c/(RK)$, be obtained using the voltage terms defined above?

a) $ZT = \dfrac{V_S}{V_T}$

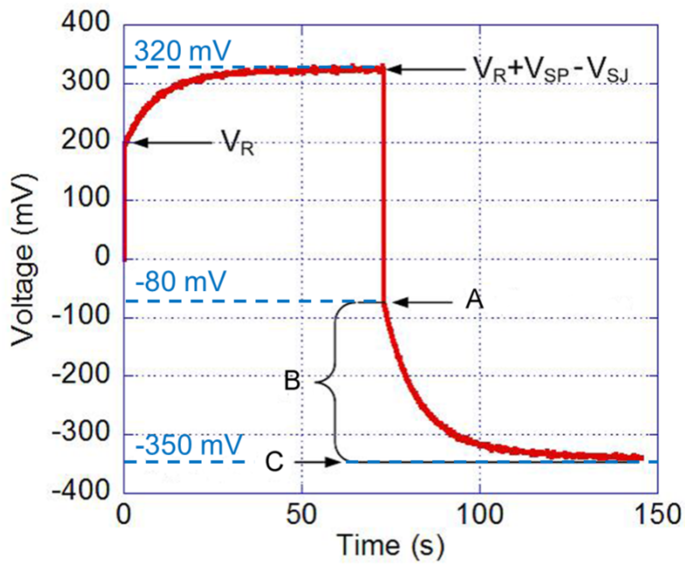
b) $ZT = \dfrac{V_{SP} + V_{SJ}}{V_T}$

c) $ZT = \dfrac{V_{SJ}}{V_R}$

d) $ZT = \dfrac{V_{SP}}{V_R}$

e) None of the above

Now, it is possible to separate each voltage term if the transient voltage across the device can be measured. The following figure shows the transient voltage response to the input current in one direction turned on at t=0, and then switched in the opposite direction at t=70 s.



1-2. Write down the expression for the three voltages, A, B, and C, shown in the figure above? Note that the ohmic voltage is almost instantaneously appearing or disappearing when the current is turned on or off, whereas the Seebeck voltage decays slowly as the temperature gradient is established with time. Also, the Peltier effect-induced voltage depends on the current polarity, whereas the Joule effect-induced voltage does not.

a) $A = V_{SP} - V_{SJ}$, $B = V_{SP}$, $C = -V_{SJ}$

b) $A = V_{SP} - V_{SJ}$, $B = 2V_{SJ}$, $C = V_{SP} - 3V_{SJ}$

c) $A = -V_R + V_{SP} - V_{SJ}$, $B = V_{SJ}$, $C = -V_R + V_{SP} - 2V_{SJ}$

d) $A = -V_R + V_{SP} - V_{SJ}$, $B = V_{SP}$, $C = -V_R - V_{SJ}$

e) $A = -V_R + V_{SP} - V_{SJ}$, $B = 2V_{SP}$, $C = -V_R - V_{SP} - V_{SJ}$

1-3. What is the figure of merit ZT of this material?

a) 0.5

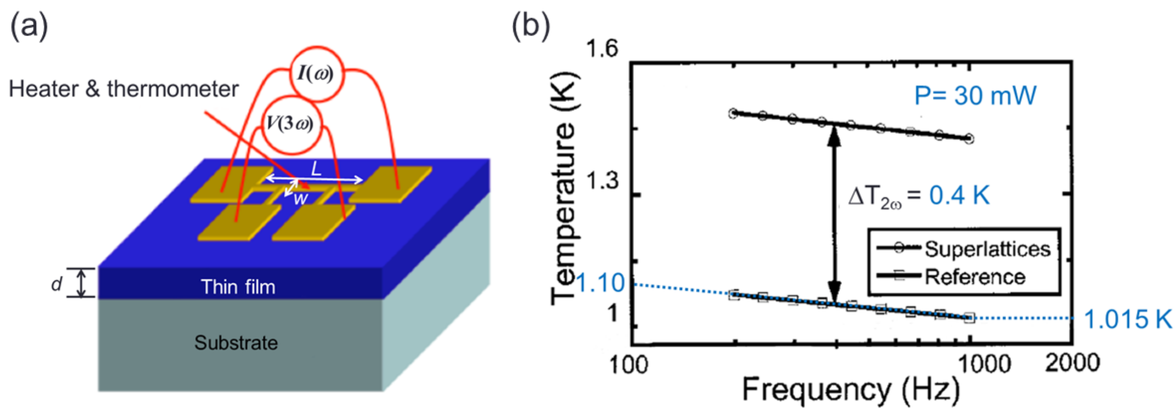
b) 0.675

c) 0.8

d) 0.975

e) 1.0

2. (3ω method) An AC current at frequency ω is applied to a metal heater line shown in the figure (a) below for measurement of the thermal conductivity of a thin film. The 3ω component of voltage is measured to obtain the temperature increase ΔT of the heater line at 2ω.



(Figure from Yang et al. APL 80, 1758 (2002))

The resulting $\Delta T_{2\omega}$ as a function of frequency is shown in the figure (b) above for a SiGe superlattice thin film sample and a reference substrate without the thin film.

2-1. Assuming that the heat conduction from the heater line through the thin film is strictly one dimensional in the cross-plane direction, calculate the thermal conductivity of the SiGe superlattice thin film using the data in figure (b). Use L = 1 mm, w = 25 µm, and d = 1 µm.

a) 2.5 W/mK

b) 3.0 W/mK

c) 3.5 W/mK

d) 4.0 W/mK

e) 4.5 W/mK

2-2. In the case of a semi-infinite substrate, the temperature increase can be approximated to the first order as a function of frequency ω to be

$$\Delta T_S = \frac{P}{\pi L \kappa_S}\left[\frac{1}{2}\ln\left(\frac{4D_S}{w^2}\right)+\eta-\frac{1}{2}\ln(2\omega)-i\frac{\pi}{4}\right], \qquad (5)$$

where κ is the thermal conductivity, D is the diffusivity, η is a constant, and subscript s denotes property of the substrate. Using the reference data in figure (b) above, calculate the thermal conductivity of the substrate. Choose the closest value. (Hint: take the derivative of both sides of Eq. (5) with respect to *log*(ω)).

a) κ_s = 30 W/mK

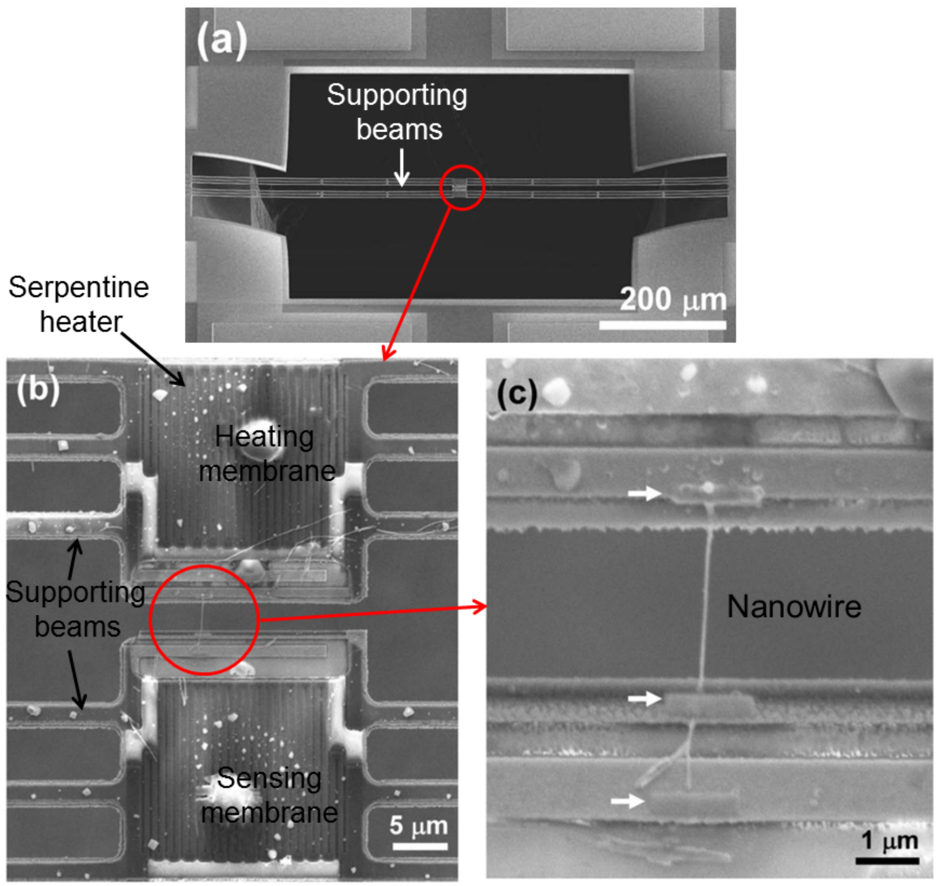
b) κ_s = 55 W/mK

c) κ_s = 130 W/mK

d) κ_s = 180 W/mK

e) κ_s = 220 W/mK

3. (Thermal measurement of individual nanowire) The device used for individual nanowire measurements consists of two adjacent thermally isolated membranes that are supported by long narrow beams as shown in the figure below. In this device, total six supporting beams are used for each membrane. An individual nanowire is placed like a bridge in between the two membranes for its measurements. Serpentine heater lines are fabricated on each membrane. These heater lines are precisely calibrated to accurately measure the membrane temperature.



(Figures from Moore *et al.* J. Appl. Phys. **106**, 034310 (2009))

3-1. Let's heat the heating membrane by applying an electric current through the electrodes on two of the supporting beams to the serpentine heater on the membrane. The Joule heating in each of the electrodes on the supporting beams is Q_l and the total heat generated on the serpentine heater is Q_h. The temperature of the heating membrane is measured to have increased by ΔT_h. The other membrane is slightly heated at the same time by ΔT_s as heat flows through the nanowire from one to the other membrane. Both membranes lose heat through the six supporting beams. Assume that membranes are uniformly heated, and the heat loss by the radiation from the nanowire surface is Q_{rad}. Also assume that all of the supporting beams are heat-sinked at the other ends at the environment temperature. Determine the thermal resistance of the six supporting beams R_b using ΔT_s, ΔT_h, Q_h , Q_l, and Q_{rad}.

a) $R_b = \dfrac{\Delta T_h - \Delta T_s}{Q_h + Q_l + Q_{rad}}$

b) $R_b = \dfrac{\Delta T_h - \Delta T_s}{Q_h + Q_l - Q_{rad}}$

c) $R_b = \dfrac{\Delta T_h + \Delta T_s}{Q_h + Q_l - Q_{rad}}$

d) $R_b = \dfrac{\Delta T_h}{Q_h - Q_l + Q_{rad}}$

e) $R_b = \dfrac{\Delta T_s}{Q_h - Q_l + Q_{rad}}$

3-2. Now assume that we know R_b. Determine the thermal resistance of the nanowire R_{NW} using ΔT_s, ΔT_h, and R_b. Also include in the calculation the two thermal contact resistances between the nanowire and the membranes, R_{c1} and R_{c2}.

a) $R_{NW} = R_b \dfrac{\Delta T_h - \Delta T_s}{\Delta T_s} - R_{c1} - R_{c2}$

b) $R_{NW} = R_b \dfrac{\Delta T_h + \Delta T_s}{\Delta T_s} - R_{c1} - R_{c2}$

c) $R_{NW} = R_b \dfrac{\Delta T_h - \Delta T_s}{\Delta T_s} + R_{c1} + R_{c2}$

d) $R_{NW} = R_b \dfrac{\Delta T_h - \Delta T_s}{\Delta T_h} - R_{c1} - R_{c2}$

e) $R_{NW} = R_b \dfrac{\Delta T_h - \Delta T_s}{\Delta T_h} + R_{c1} + R_{c2}$

3-3. Choose correct statements about potential parasitic heat losses in the measurement.

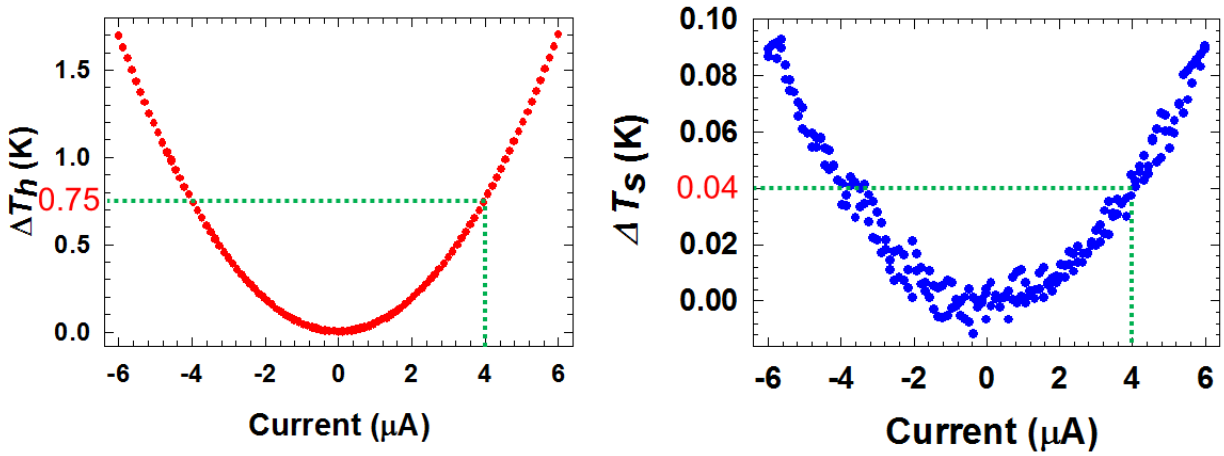
a) Thermal resistance of nanowire is underestimated if radiation loss from the nanowire surface is not taken into account.

b) Radiation loss can be negligibly small if the nanowire is sufficiently thick and short.

c) Thermal contact resistances between nanowire and membranes reduce the actual temperature gradient across the nanowire, and create non-uniform temperature on the portion of the nanowire that is in contact with the membrane surface.

d) The nanowire thermal resistance is overestimated unless the thermal contact resistances are accurately quantified and added.

e) All of the above



(Figures from Shi *et al.* J. Heat Transfer **125**, 811 (2003))

3-4. The above figures show the temperature increases of the heating membrane and the sensing membrane as a function of heater current. This measurement is done with a 148 nm-diameter single-wall carbon nanotube (SWCN) bundle at 55 K. The resistance of the serpentine heater on the heating membrane is 2.00 kΩ, and the resistance of one electrode on a supporting beam is 0.47 kΩ. The length of the SWCN bundle is 3 μm. Using the temperature increase values with heater current at 4 μA from the figures, calculate the total thermal resistance of the supporting beams R_b, and the thermal conductivity of the SWCN bundle κ_{SWCN} at 55 K. (Ignore the parasitic heat losses discussed in the previous problems.)

a) $R_b = 1.0 \times 10^7$ K/W, $\kappa_{SWCN} = 0.49$ W/mK

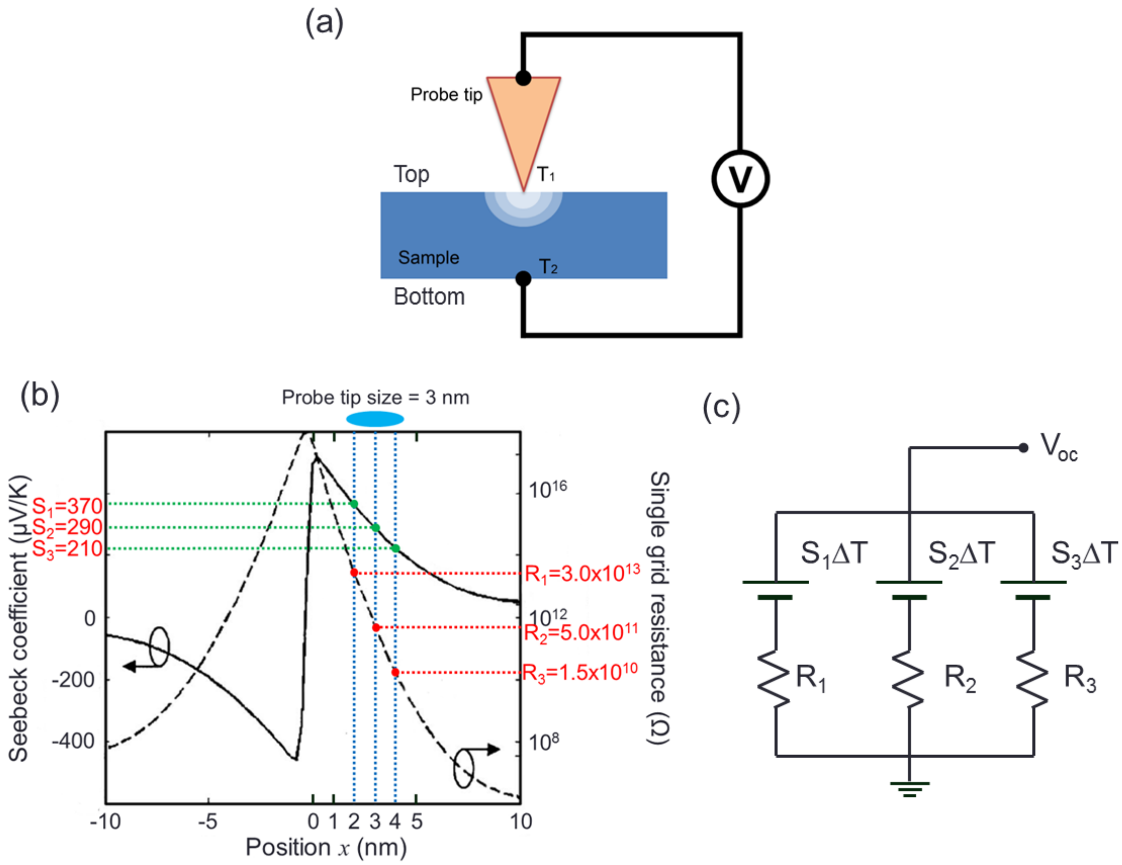
b) $R_b = 1.0 \times 10^7$ K/W, $\kappa_{SWCN} = 0.98$ W/mK

c) $R_b = 2.0 \times 10^7$ K/W, $\kappa_{SWCN} = 0.49$ W/mK

d) $R_b = 2.0 \times 10^7$ K/W, $\kappa_{SWCN} = 0.98$ W/mK

e) $R_b = 2.0 \times 10^7$ K/W, $\kappa_{SWCN} = 1.96$ W/mK

4. (Scanning thermal probe method) Scanning thermal probe method is very useful to measure the two-dimensional variation of Seebeck coefficient on an inhomogeneous sample surface with a high spatial resolution. When a cold tip is in contact with a heated substrate, a temperature gradient ΔT across the sample is created as shown in figure (a) below. The voltage ΔV across the sample is then measured to obtain the local Seebeck coefficient at the probe tip position using $S = \Delta V/\Delta T$.



In order to investigate uncertainty in the measurement of local Seebeck coefficient induced by a finite size of the probe tip, consider a p-n junction device that has variation of Seebeck coefficient and single grid local resistance as a function of horizontal position near the p-n junction as shown in figure (b). Note that the local resistance varies much more rapidly with position than the local Seebeck coefficient does. A 3 nm-diameter probe tip is placed on position x = 3 nm. Assuming that the sample is homogeneous in the cross-plane direction and the temperature gradient is purely one-dimensional in that direction, the measured open-circuit voltage V_{oc} can be modeled as an electric circuit of multiple resistors and voltage sources in parallel connection. For simplicity we only consider three parallel voltage sources touching the tip at positions 2, 3 and 4nm as shown in figures (3)(b) and (c).

4-1. Use the values of Seebeck coefficient and resistance shown in figure (b) in the electric circuit model in figure (c), and solve the Kirchoff's law for the circuit to find the Seebeck coefficient value measured by the probe tip. See how the measured Seebeck coefficient is different from the actual value at the center of the probe tip at x =3 nm.

a) 212.4 μV/K
b) 252.4 μV/K
c) 292.4 μV/K
d) 324.4 μV/K
e) 368.4 μV/K

4-2. Which one is closest to the measured Seebeck coefficient value, and why?

a) S_1, because R_1 is much larger than the other two resistances.
b) $(S_1+S_2)/2$, because R_3 is much smaller than the other two resistances.
c) S_2, because the probe tip is centered at the position of R_2.
d) $(S_2+S_3)/2$, because R_1 is much larger than the other two resistances.
e) S_3, because R_3 is much smaller than the other two resistances.

5. (Raman spectroscopy for temperature measurement) When a specimen is irradiated with a laser beam, the photons of the beam undergo inelastic scattering due to lattice vibration specific to the material of the specimen, so that the frequency of the photons shifts by an amount equivalent to the optically active phonon modes. There are two types of Raman shift: Stoke shift due to excitation of lattices in ground vibrational states, and Anti-Stoke shift due to excitation of lattice in excited vibrational states as shown in the figure (a) below. The population of electrons in each state is governed by the Boltzmann distribution, and the Raman scattering rates are proportional to the forth power of the excitation frequency or wavenumber. Therefore, the anti-Stoke/Stoke intensity ratio is given by

$$\frac{I_{AS}}{I_S} = \frac{(\omega_0 - \omega_1)^4}{(\omega_0 + \omega_1)^4} \exp\left(- \frac{hc\omega_1}{k_B T} \right), \tag{5-1}$$

where I_{AS} and I_S are the anti-Stokes and Stokes intensities, respectively, arising from a vibrational wavenumber shift ω_1, with the use of an excitation light source of wavenumber ω_0. c = 3.0 × 10^8 (m/s) is the speed of light, k_B = 1.38 × 10^{-23} ($m^2kg/(s^2K)$) is the Boltzmann constant, h = 6.626 × 10^{-34} (m^2kg/s) is the Planck constant, and T is the absolute temperature.

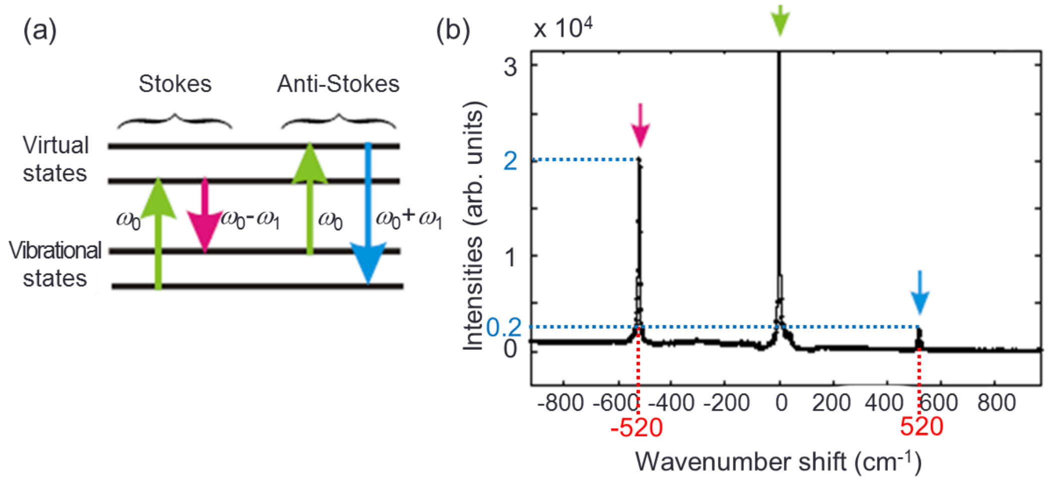


Figure (b) shown above presents the Stokes and Anti-Stokes intensities obtained from a silicon sample with an excitation by a 632.8 nm He-Ne laser. Find the absolute temperature of the sample using (5-1).

a) 267.3 K

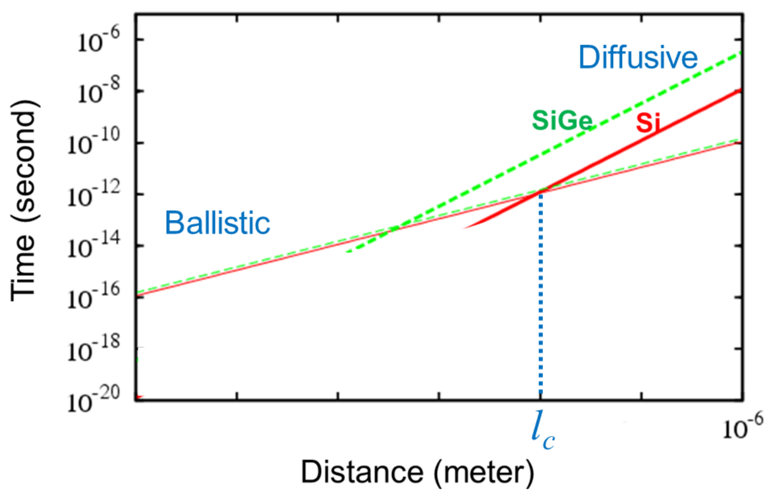
b) 297.3 K

c) 337.3 K

d) 367.3 K

e) 413.3 K

6. (Ballistic and diffusive thermal transport) The Fourier law of heat conduction describes transient transport of heat in the diffusive transport limit. In the one-dimensional diffusive transport of heat, the traveling time to reach a distance l is inversely proportional to the thermal diffusivity of the medium D, and proportional to l^2 such that $t_d = l^2/D$. In a very short length scale where phonon scattering is negligibly small, the transport is ballistic. The traveling time of heat (energy) for a distance l in the ballistic transport limit can be obtained with a constant speed that can be represented by the average speed of sound in the medium. One can define a characteristic length of a material, where ballistic transport starts to become important, by equating the ballistic traveling time with the diffusive one as shown in the figure below. Calculate the characteristic length l_c for silicon crystal at room temperature. Thermal diffusivity of silicon is $D = 8.8 \times 10^{-5}$ m^2/s and the speed of sound in silicon is $v_s = 8.433 \times 10^3$ m/s at room temperature. Also, what is the characteristic time t_0 corresponding to the length l_c for silicon at room temperature?



a) $l_c = 1$ nm, $t_0 = 0.12$ ps

b) $l_c = 10$ nm, $t_0 = 1.2$ ps

c) $l_c = 50$ nm, $t_0 = 12$ ps

d) $l_c = 100$ nm, $t_0 = 12$ ps

e) $l_c = 1$ μm, $t_0 = 120$ ps