1

Shown below on the left is a figure obtained by measuring the macroscopic expansion of length of a rod of pure gold, $\frac{\Delta I}{I_0}$, as a function of temperature and simultaneously using x-ray diffraction to measure $\frac{\Delta a}{a_0}$, where a is the lattice parameter of the unit cell. From this data set the authors obtained the following expression for the concentration of vacancies as a function of temperature

$$\frac{\Delta N}{N} = \frac{N_V}{N} = \exp(1.0)\exp\left(-\frac{0.94\,eV}{kT}\right)$$

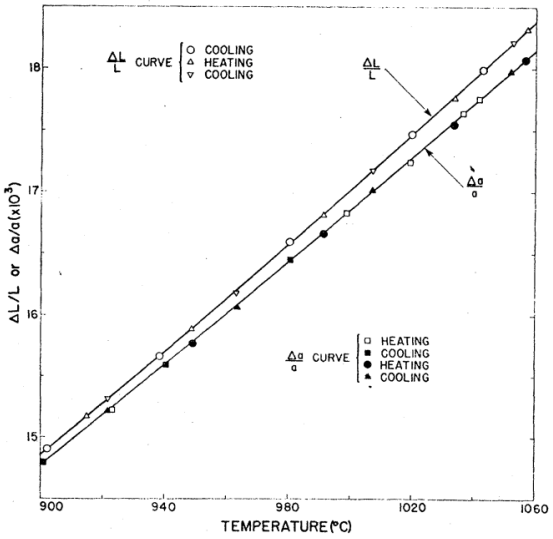

FIG. 2. Measured length expansion $\Delta L/L$ and lattice parameter expansion $\Delta a/a$ versus temperature in the interval 900°–1060°C. $\Delta L/L$ becomes larger than $\Delta a/a$ at the highest temperatures corresponding to the thermal generation of lattice vacancies. The melting temperature of gold is 1063°C.

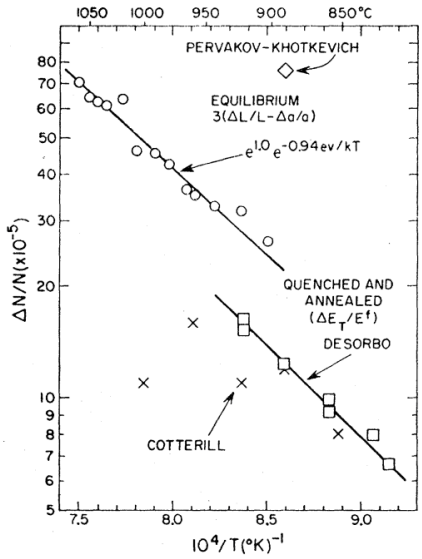

FIG. 3. Atomic fraction of vacant lattice sites $\Delta N/N$ versus inverse temperature in gold. The present equilibrium values of $\Delta N/N = 3(\Delta L/L - \Delta a/a)$ were computed directly from pairs of corresponding expansion measurements. DeSorbo[3] measured total

a

Calculate the fraction of vacant sites in gold at 950°C. Plot this value on Fig 3 noting the vertical axis is logarithmic.

✓ **Answer**

$$\exp(1.0)\exp\left(-\frac{0.94\,eV}{kT}\right)$$
$$= \exp(1.0)\exp\left(-\frac{0.94}{8.6173\times10^{-5}(950+273.15)}\right)$$
$$= 3.64\times10^{-4}$$

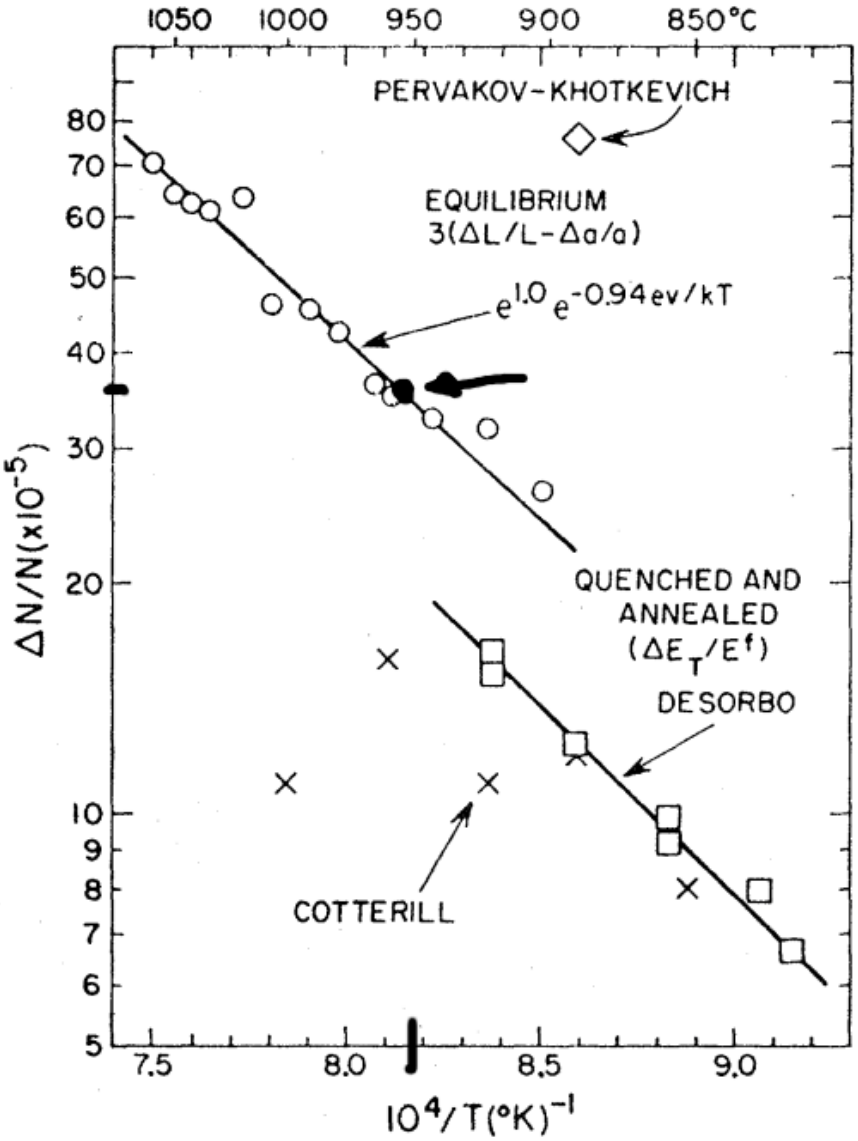

FIG. 3. Atomic fraction of vacant lattice sites $\Delta N/N$ versus inverse temperature in gold. The present equilibrium values of $\Delta N/N = 3(\Delta L/L - \Delta a/a)$ were computed directly from pairs of corresponding expansion measurements. DeSorbo[3] measured total

b

Assuming the density of gold is $18.4\ g/cm^3$ at $950^\circ C$, and using the result from Part a, calculate the number of vacancies in $1\ cm^3$ of gold at $950^\circ C$.

✓ **Answer**

$N_V = 3.64 \times 10^{-4} N$

$N = \frac{18.4(6.023 \times 10^{23})}{197}$

$N_V = 2.03 \times 10^{19}$ sites

c

On Fig 2, the authors have superimposed data obtained during heating and also during cooling back down. Explain what they are demonstrating by showing that they get the same result in either direction.

✓ **Answer**

The data points on the graph all fall upon the same line whether it be heating or cooling, sticking very strictly to the linear fit, without lag or variance. This also shows a full recovery across heating and cooling.

2

Calculate the number of vacancies per cubic centimeter in iron at $850^{\circ}C$. The energy for vacancy formation is $1.08\ eV/atom$. The density and atomic weight for Fe are $7.65\ g/cm^3$ and $55.85\ g/mol$, respectively.

✓ **Answer**

$N = 7.65\left(\frac{6.02\times10^{-23}}{55.85}\right)$
$N_V = N\exp\left(-\frac{1.08}{8.673\times10^{-5}(1123.15)}\right)$
$N = 1.17\times10^{18}\ cm^{-3}$

3

In ionic ceramics, Shottky defects are described a stoichiometric set of vacancies.
Define the term stoichiometric.
Describe a stoichiometric set of vacancies for MgO and for Al_2O_3.

✓ **Answer**

Reactants are in a set ratio in order to produce a certain product. In a Shottky defect, that same ratio is missing from a lattice.

MgO: 1Mg and 1O vacancy
Al_2O_3: 2Al and 3O vacancy

4

Considering the Hume-Rothery rules (described in section 5.4) and the data in the following table:

Choose which of these elements would you expect to form the following with copper:

Element	Atomic Radius (nm)	Crystal Structure	Electronegativity	Valence
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Pt	0.1387	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

a

A substitutional solid solution having complete solubility

✓ **Answer**

$Cu \rightarrow Ni, Pd, Pt$

All:

1. Radii match
2. Same crystal structure
3. Same electronegativity and same valence

b

A substitutional solid solution of incomplete solubility

✓ **Answer**

$Cu \rightarrow Ag, Al, Co, Cr, Fe, Zn$

1. Valence electrons don't match

2. Valence electrons don't match
3. Different Crystal Structure
4. Different Crystal Structure
5. Different Crystal Structure
6. Different Crystal Structure

c

An interstitial solid solution

✓ **Answer**

$Cu \rightarrow C, H, O$

1. Radii do not match, Cu is significantly bigger

5

Explain how the strongly directional nature of covalent bonding would affect the energy cost of forming and moving dislocations in a material like silicon.

✓ **Answer**

Dislocation formation in an area requires bonds of an atom to be bent or moved away from their original state. When the bond is covalent, there is a huge energy cost required to break or move these bonds.