I. Thermoelectric material discovery

The thermoelectric effect enables the direct conversion of heat into electricity and vice versa, which has received intensive interest for powering IoT devices and cooling applications. Discovering materials with an intrinsically low lattice thermal conductivity κlat is an important route for decoupling these interrelated thermoelectric parameters and therefore achieving high thermoelectric performance. The conventional synthetic approach used long-term has been based largely on laboratory trial and error, or complex quantum calculations. In this study, we proposed a new crystallographic parameter, namely the site occupancy factor, as an effective indicator to identify a material catalogue with low κlat using the REST-API framework. In a representative material, Cu_6Te_3S, which contains Cu with partial occupancy, an amorphous thermal conductivity was observed and, more importantly, the thermoelectric performance can be further enhanced by Ag alloying on the Cu site. The corresponding phonon mechanism of low κlat was attributed to the anharmonic and anisotropic vibration of the Cu atom, the ionic bond feature around the Cu atom, and the global weak bonding. Our study offers fresh insights into discovering materials with low κlat for thermoelectric applications.

(1) Direct conversion of heat into electricity and vice versa is enabled by

(a) Amorphous thermal conductivity
(b) Global weak bonding
(c) Anharmonic vibration
(d) Thermoelectric effect

(2) In the representative material Cu_6Te_3S

(a) Amorphous thermal conductivity is observed
(b) Strong global bonding is observed
(c) Phonons are harmonic and isotropic
(d) Around Cu, the bond is metallic

(3) What properties are needed for achieving high thermoelectric performance?

(a) Metallic bonding
(b) Low lattice thermal conductivity
(c) High lattice thermal conductivity
(d) No lattice vibration

(4) Thermoelectric effect is useful in applications of

(a) IoT and cooling applications
(b) Superconductivity
(c) REST-API framework
(d) Crystallography

(5) The phonon mechanism of low lattice thermal conductivity is

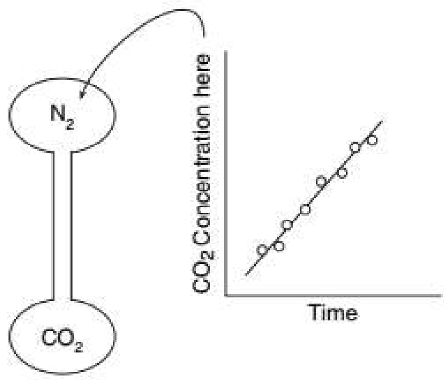
(a) solely due to the anisotropic vibration of Cu atoms

(b) solely due to the anharmonic vibration of Cu atoms
(c) solely due to the substitution of Cu atoms by Ag
(d) among other things, also due to ionic bond feature around the Cu atom, and the global weak bonding

II. Models for diffusion – the two basic models

Adapted from E. L. Cussler, "Diffusion: Mass Transfer in Fluid Systems", 3rd Ed., Cambridge (2009)

To describe the process of diffusion in fluid systems, we first imagine two large bulbs connected by a long thin capillary tube (*shown in the figure here*). The bulbs are at constant temperature and pressure and are of equal volumes. However, one bulb contains carbon dioxide, and the other is filled with nitrogen. To find how fast these two gases will mix, we measure the concentration of carbon dioxide in the bulb that initially contains nitrogen. We make these measurements when only a trace of carbon dioxide has been transferred, and we find that the concentration of carbon dioxide varies linearly with time. From this, we know the amount transferred per unit time.



We want to analyze this amount transferred to determine physical properties that will be applicable not only to this experiment but also in other experiments. To do this, we first define the flux:

$$(CO_2\ flux) = \left(\frac{amount\ of\ gas\ removed}{time\ \times\ area\ of\ capillary\ tube}\right) \qquad \textit{Equation 1}$$

In other words, if we double the cross-sectional area, we expect the amount transported to double. Defining the flux in this way is a first step in removing the influences of our particular apparatus and making our results more general. We next assume that the flux is proportional to the gas concentration:

$$(CO_2\ flux) = k \cdot (CO_2\ concentration\ difference) \qquad \textit{Equation 2}$$

The proportionality constant k is called a mass transfer coefficient. Its introduction signals one of the two basic models of diffusion. Alternatively, we can recognize,

$$(CO_2\ flux) = D\left(\frac{CO_2\ concentration\ difference}{capillary\ tube\ length}\right) \qquad \textit{Equation 3}$$

The new proportionality constant D is the diffusion coefficient. Its introduction implies the other model for diffusion, the model often called Fick's law.

1) Assuming ideal behaviour (PV=nRT), can we estimate the initial molar ratios of the amounts of CO_2 and N_2 gases, (moles of CO_2): (moles of N_2), contained in the respective bulbs at the beginning of the experiment?
A: Cannot say, since temperature and pressure are not known
B: Equimolar ratio of 1:1

C: In the ratio of their respective molecular weights, $M_{CO_2}: M_{N_2}$
D: In the ratio of their respective virial coefficients, $B_{CO_2}: B_{N_2}$

2) The correct units for the flux of CO_2 should be,
A: $\frac{moles\ of\ CO_2}{m^3 \cdot s}$
B: $\frac{number\ of\ CO_2\ molecules}{s}$
C: $\frac{number\ of\ CO_2\ molecules}{m^2 \cdot s}$
D: $\frac{moles\ of\ CO_2}{m^2}$

3) For diffusion across a thin film of stagnant fluid of thickness, δ, the mass transfer coefficient, k, can be interpreted as,
A: $k = \frac{D}{\delta}$
B: $k = \frac{D}{\delta^2}$
C: $k = \frac{\delta}{D}$
D: $k = D\delta$

4) Equation 2 represents a model of diffusion and is analogous to the Ohm's law, $I = V/R$, where V is the voltage (or potential difference), I is the current (or flux of electrons times area), and R is the electrical resistance. Then, the mass transfer coefficient, k, can be understood to be analogous to,
A: current
B: resistance
C: reciprocal of the resistance
D: reciprocal of the current

5) Industrial pollutants in Agra can cause significant corrosion of the marble in Taj Mahal. You want to study how these pollutants penetrate marble. Which diffusion model should you use, the mass transfer coefficients model (Equation 2) or the diffusion coefficients model (Equation 3)?
A: Equation 3 because it predicts pollutant concentration versus position in the marble
B: Equation 2 because it correlates how much pollutant enters the marble
C: Equation 2 because only the average pollutant concentration in the marble is required
D: Equation 3 because it can be used to estimate the molecular size of the pollutant molecule

I. Population distribution on a plane

Clark and Evans, Ecology, Vol. 35, 1954, No. 4, pp. 445-453

The measure of spacing which we propose is a measure of the manner and degree to which the distribution of individuals in a population on a given area departs from that of a random distribution. Some clarification of what is meant by a "random distribution" is therefore desirable. In a random distribution of a set of points on a given area, it is assumed that any point has had the same chance of occurring on any sub-area as any other point, that any sub-area of specified size has had the same chance of receiving a point as any other sub-area of that size, and that the placement of each point has not been influenced by that of any other point. Thus, randomness as here employed is a spatial concept, intimately dependent upon the boundaries of the space chosen by the investigator. A set of points may be random with respect to a specified area but decidedly non-random with respect to a larger space which includes the specified area. For meaningful results, therefore, the areas selected for investigation should be chosen with care.

The distance from an individual to its nearest neighbor, irrespective of direction, provides the basis for this measuring of spacing. A series of such distances is measured in a given population, using all of the individuals present or a randomly selected sample, and the value of the mean distance to nearest neighbor is obtained for this set of observations. The mean distance to nearest neighbor that would be expected if the individuals of that population were randomly distributed is also calculated. The ratio of the observed mean distance to the expected mean distance serves as the measure of departure from randomness. The ratios that have been calculated for two or more populations can be directly compared with one another, as a measure of their relative departure from random expectation.

Qn1. Consider the definition of randomness given in the passage above. Which of the following statements is false?

A. Whether a set of points are random or not depends on the area selected.
B. The departure from randomness is defined in terms of a ratio of mean distances.
C. The area for analysis can be chosen arbitrarily.
D. Randomness employed here is a spatial concept.

Qn2. The authors of this study define random distribution of points in terms of

A. Density of points
B. Spacing between points
C. Area occupied by the points
D. Shape of the chosen area

Qn3. What is considered as a measure of spacing between points distributed over a selected area?

A. Mean of the distance between a point and all other points
B. Mean of the distance between nearest neighbor for all points in the selected area
C. Median of the distance between a point and all other points
D. Median of the distance between nearest neighbor for all pointes in the selected area

Qn4. Consider a distribution of points for which the ratio of the observed mean distance to the expected mean distance is R. Which of the following interpretation regarding the value of R is false?

A. $R = 1$ implies distribution is completely random
B. R may be greater than 1
C. $R \sim 0$ implies maximum aggregation

D. R value of 2 would mean that points are much closer than they would have been in a random distribution

Qn5. Consider a simple case of 10 particles distributed over an area of 1 mm^2. The measured distance with nearest neighbor for each particle is given in the following table. What would be the ratio R for this distribution? Please note that the mean nearest neighbor distance for randomly distributed particles is given by: $\frac{1}{2\sqrt{\rho}}$, where ρ is the number of particles per unit area.

Particle	1	2	3	4	5	6	7	8	9	10
NND (mm)	0.1	0.2	0.5	0.2	0.1	0.4	0.3	0.3	0.2	0.1

A. 2.3
B. 2.5
C. 1.5
D. 1.3