In-Class Exercise
Diffusion Coefficient
SOLUTION

1. The diffusion coefficient of oxygen ions in cubic zirconia was found experimentally to be $D_o = 3.4\times10^{-3}\,\frac{cm^2}{s}$

   $Q, E_A = 0.99eV$

Reference: M. Kilo, C. Argirusis, G. Borchardt, and R.A. Jackson, "Oxygen diffusion in yttria stabilized zirconia – experimental results and molecular dynamics calculations," *Phys. Chem. Chem. Phys.*, **5** (2003) 2219-2224.

Each team member calculate D for a different temperature (300-1250K) and generate a plot.

$$D_{300} = D_o \exp\left\{-\frac{Q}{kT}\right\} = 3.4\times10^{-3}\cdot cm^2/s \bullet \exp\left\{-\frac{0.99\cdot eV}{86.20\times10^{-6}\cdot eV/K \bullet 300\cdot K}\right\}$$

$$= 8.0\times10^{-20}\cdot cm^2/s$$

$$D_{500} = D_o \exp\left\{-\frac{Q}{kT}\right\} = 3.4\times10^{-3}\cdot cm^2/s \bullet \exp\left\{-\frac{0.99\cdot eV}{86.20\times10^{-6}\cdot eV/K \bullet 500\cdot K}\right\}$$

$$= 3.6\times10^{-13}\cdot cm^2/s$$

$$D_{1000} = D_o \exp\left\{-\frac{Q}{kT}\right\} = 3.4\times10^{-3}\cdot cm^2/s \bullet \exp\left\{-\frac{0.99\cdot eV}{86.20\times10^{-6}\cdot eV/K \bullet 1000\cdot K}\right\}$$

$$= 3.5\times10^{-8}\cdot cm^2/s$$

$$D_{1250} = D_o \exp\left\{-\frac{Q}{kT}\right\} = 3.4\times10^{-3}\cdot cm^2/s \bullet \exp\left\{-\frac{0.99\cdot eV}{86.20\times10^{-6}\cdot eV/K \bullet 1250\cdot K}\right\}$$

$$= 3.5\times10^{-7}\cdot cm^2/s$$