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Appendix

The jump frequency has been developed very generally by Vineyard[12] as

$$\Gamma = \left(\frac{\kappa T}{2\pi m}\right)^{1/2} \int_\sigma e^{-\varphi/RT}\, d\sigma \Big/ \int_A e^{-\varphi/RT}\, dA \quad (1a)$$

where φ is the potential energy for all the atoms in the crystal, A is an appropriate phase space volume taken at an atom neighboring a vacancy, and σ is an appropriate hypersurface taken at the saddle configuration of the jump. To a first approximation, A is the same for different jump directions in anisotropic systems; hence anisotropy must arise mostly from different σ_k for different jump types k. Thus (1a) becomes

$$\Gamma_k = \left(\frac{\kappa T}{2\pi m}\right)^{1/2} \int_{\sigma k} e^{-\varphi/RT}\, d\sigma_k \Big/ \int_A e^{-\varphi/RT}\, dA \quad (2a)$$

Following Girifalco and Grimes,[11] expand φ in terms of the strains, ϵ_i, to first order, and define

$$m_i{}^k = \left\langle \frac{\partial \varphi}{\partial \epsilon_i} \right\rangle_A - \left\langle \frac{\partial \varphi}{\partial \epsilon_i} \right\rangle_{\sigma k} \quad (3a)$$

where $\langle\ \rangle$ denotes the usual statistical averages over A or σ_k. Now (2a) becomes

$$\Gamma_k(\epsilon) = \Gamma_k(0) \exp\left[\frac{1}{RT} \sum_i m_i{}^k \epsilon_i\right] \quad (4a)$$

The vacancy concentration may be written analogously as

$$n_v(\epsilon) = n_v(0) \exp\left[\frac{1}{RT} \sum w_i \epsilon_i\right] \quad (5a)$$

where

$$w_i = \left\langle \frac{\partial \varphi_0}{\partial \epsilon_i} \right\rangle - \left\langle \frac{\partial \varphi_v}{\partial \epsilon_i} \right\rangle \quad (6a)$$

Here φ_0 and φ_v are the potential energies of the crystal without and with a vacancy, respectively. Note that w_i is independent of direction k.

From the zero strain expression $D_k(0) = \gamma_k a_k{}^2 n_v \cdot (0)\Gamma_k(0)$, the diffusion coefficient of the strained crystal is

$$D_k(\epsilon) = D_k(0)(1 + \epsilon_k)^2 \exp\left[\frac{1}{RT} \sum_i M_i{}^k \epsilon_i\right] \quad (7a)$$

where

$$M_i{}^k = m_i{}^k + w_i \quad (8a)$$

The only unknown quantities in (7a) are the $M_i{}^k$. These may be found from

$$\frac{\partial \ln D_k(\epsilon)}{\partial \epsilon_i} - \frac{2\partial \ln (1 + \epsilon_k)}{\partial \epsilon_i} = \frac{M_i{}^k}{RT} \quad (9a)$$

From elasticity theory we write $\epsilon_i = \sum_j s_{ij} P_j$, where the stress, P_j, is a force per unit area (pressure), and the s_{ij} are constants. Then (9a) becomes

$$\sum_j \frac{\partial \ln D_k(P)}{\partial P_j} - 2\sum_j s_{kj}/1 + \sum_j s_{kj} P_j = \sum_{i,j} \frac{M_i{}^k s_{ij}}{RT} \quad (10a)$$

From the Zener formalism[22] we have

$$\frac{\partial \ln D_k(P)}{\partial P} - 2\sum_j s_{kj} = \frac{1}{RT} \sum_{i,j} \Delta V_{ij}{}^* - \sum_j s_{ij} \quad (11a)$$

so that

$$\sum_{i,j} \Delta V_{ij}{}^* = \sum_i (M_i{}^k + \gamma RT \delta_{ik}) s_i \quad (12a)$$

where δ_{ik} is the Kronacker delta, and we have set $1 + \sum_j s_{ij} P_j$ equal to unity, and where $\sum_j s_{ij} = S_i$. Summing (12a) over j gives ΔV^k in terms of strain components, $\Delta V_i{}^k$, while a sum over i gives the stress components $\Delta V_j{}^k$. Hydrostatic pressure measurements give only their sums so neither set is more significant.

The $M_i{}^k$ will have the same relations as the s_{ij}. For example, for nonshear stresses, the x and y axes of tetragonal crystals are indistinguishable so that only five independent $M_i{}^k$ remain, for instance, $M_1{}^1$, $M_2{}^1$, $M_3{}^1$, $M_1{}^3$, and $M_3{}^3$. Hence, five uniaxial and/or hydrostatic diffusion experiments are required to determine fully the $M_i{}^k$ in this case.