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--- Diffusion in Minerals and Melts ---

## Chapter 2: Diffusion in Minerals and Melts: Theoretical Background

 Pages 5-59
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In Appendix 1 (pages 58-59), the equations given for the diffusivity along any direction (the first two lines below ea. A2, first line below eq. A3, and fifth line below eq. A6) in an anisotropic crystal only applies to the special case when that direction is parallel to the concentration gradient. In general cases, the equation along any direction $\mathbf{v}$ is:

$$
D_{\mathbf{v}}=-\frac{\mathbf{J} \cdot \mathbf{v}}{(\nabla C) \cdot \mathbf{v}}=\frac{D_{1} \frac{\partial C}{\partial x} \cos \theta_{1}+D_{2} \frac{\partial C}{\partial y} \cos \theta_{2}+D_{3} \frac{\partial C}{\partial z} \cos \theta_{3}}{\frac{\partial C}{\partial x} \cos \theta_{1}+\frac{\partial C}{\partial y} \cos \theta_{2}+\frac{\partial C}{\partial z} \cos \theta_{3}},
$$

where $C$ is the concentration, $\mathbf{v}$ is the direction vector along which the diffusivity is evaluated, $\mathbf{J}$ is the diffusive flux (vector), $\nabla C$ is the concentration gradient (vector), $\theta_{1}$, $\theta_{2}$, and $\theta_{3}$ are the angles between $\mathbf{v}$ and the respective principal diffusion axes (defined as $x, y$ and $z$ directions), and $D_{1}, D_{2}$, and $D_{3}$ are the principal diffusivities along the 3 principal axes, which for orthorhombic systems are the same as the crystallographic directions $a, b$ and $c$. For hexagonal, tetragonal and trigonal systems, $D_{1}=D_{2}$. For glasses and crystals of cubic systems, $D_{1}=D_{2}=D_{3}$.

For two special cases, the above equation can be simplified.
If the concentration gradient $\nabla C$ is parallel to $\mathbf{v}$, the above can be simplified as: $D_{\mathbf{v}}=D_{1} \cos ^{2} \theta_{1}+D_{2} \cos ^{2} \theta_{2}+D_{3} \cos ^{2} \theta_{3}$, which is the equation given in the Appendix.

If the diffusive flux $\mathbf{J}$ is parallel to $\mathbf{v}$, the above can be simplified as:

$$
\frac{1}{D_{\mathbf{v}}}=\frac{\cos ^{2} \theta_{1}}{D_{1}}+\frac{\cos ^{2} \theta_{2}}{D_{2}}+\frac{\cos ^{2} \theta_{3}}{D_{3}} .
$$

