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MR42A-03: A Study of Defect Behavior in Almandine Garnet

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Transport and diffusion in crystals are controlled by defects. However, a good understanding of the defect types in many silicates, including garnet, is not at hand. We undertook a study on synthetic almandine, ideal end-member $\text{Fe}_3\text{Al}_2\text{Si}_3\text{O}_{12}$, to better understand its precise chemical and physical properties and defect behavior. Crystals were synthesized at high pressures and temperatures under different f_{O_2} conditions using various starting materials with H_2O and without. The almandine obtained came in polycrystalline and single-crystal form. The synthetic reaction products and crystals were carefully characterized using X-ray powder diffraction, electron microprobe and TEM analysis and with ^{57}Fe Mössbauer, UV/VIS single-crystal absorption and IR single-crystal spectroscopy.

Various possible intrinsic defects, such as the Frenkel, Schottky and site-disorder types, along with Fe^{3+} , in both synthetic and natural almandine crystals, were analyzed based on model defects expressed in Kröger-Vink notation. Certain types of minor microscopic- to macroscopic-sized precipitation or exsolution phases, including some that are nanosized, that are observed in synthetic almandine (e.g., magnetite), as well as in more compositionally complex natural crystals (e.g., magnetite, rutile, ilmenite), may result from defect reactions. An explanation for their origin through minor amounts of defects in garnet has certain advantages over other models that have been put forth in the literature that assume strict garnet stoichiometry for their formation and/or open-system atomic transport over relatively long length scales.

Physical properties, including magnetic, electrical conductivity and diffusion behavior, as well as the color, of almandine are also analyzed in terms of various possible model defects. It is difficult, if not impossible, to synthesize stoichiometric end-member almandine, $\text{Fe}_3\text{Al}_2\text{Si}_3\text{O}_{12}$, in the laboratory, as small amounts of extrinsic OH^- and/or Fe^{3+} defects, for example, are typically present depending on the synthesis route. The nature of possible nonstoichiometry in synthetic almandine and natural almandine-rich crystals is discussed and compared.