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Can high pressure I-II transitions in semiconductors be affected by plastic flow and nanocrystal precipitation in phase I? B. A. WEINSTEIN, SUNY at Buffalo, Physics Dept., Buffalo, NY 14260 USA, G. P. LINDBERG, Rochester Precision Optics, W. Henrietta, NY 14586 USA — Pressure-Raman spectroscopy in ZnSe and ZnTe single crystals reveals that Se and Te nano-crystals (NCs) precipitate in these II-VI hosts for pressures far below their I-II phase transitions.[1] The inclusions are evident from the appearance and negative pressure-shift of the A1 Raman peaks of Se and Te (trigonal phase). The Se and Te NCs nucleate at dislocations and grain boundaries that arise from pressure-induced plastic flow. This produces chemical and structural inhomogeneities in the zincblende phase of the host. At substantially higher pressures, the I-II transition proceeds in the presence of these inhomogenities. This can affect the transition's onset pressure P_t and width ΔP_t, and the occurrence of metastable phases along the transition path. Precipitation models in metals show that nucleation of inclusions depends on the Peierls stress τ_p and a parameter α related to the net free energy gained on nucleation. For favorable values of τ_p and α, NC precipitation at pressures below the I-II transition could occur in other compounds. We propose criteria to judge whether this is likely based on the observed ranges of τ_p in the hosts, and estimates of α derived from the cohesive energy densities of the NC materials. One finds trends that can serve as a useful guide, both to test the proposed criteria, and to decide when closer scrutiny of phase transition experiments is warranted, e.g., in powders where high dislocation densities are initially created. [1] G. P. Lindberg, et. al., Phys. Status Solidi B 250, 711 (2013)

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