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TI: Electron Density Distributions for Millerite, Vaesite, Heazlewoodite and Ni metal: A Case for the Importance of NiNi Bond Paths for Electron Transport
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AB: Bond paths and the bond critical point properties have been calculated for the bonded interactions comprising the Ni sulfide minerals millerite, vaesite and heazlewoodite and Ni metal. The experimental NiS bond lengths decrease linearly as the magnitudes of the properties each increases in value. Bond paths exist between the Ni atoms in heazlewoodite and millerite for NiNi separations that match the shortest separation in Ni metal, an indicator that the Ni atoms are bonded. Bond paths also exist between the Ni atoms in bulk Ni metal. In addition, the bcp properties of the bonded interactions in Ni metal are virtually the same as those in heazlewoodite and millerite. In contrast, NiNi bond paths are absent in vaesite where the NiNi separations are 60% greater than those in Ni metal. The bcp properties for the NiNi bonded interactions scatter along protractions of the NiS bond length-bcp property trends, suggesting that the two bonded interactions have similar characteristics. NiNi bond paths radiate throughout Ni metal and the metallic heazlewoodite structures as continuous networks whereas the NiNi paths in millerite are restricted to isolated Ni_3 rings. Electron transport in Ni metal and heazlewoodite is pictured as occurring along the bond paths, which behave as networks of atomic size wires that radiate in a contiguous circuit throughout the two structures. Unlike heazlewoodite, the electron transport in millerite is pictured as involving a cooperative hopping of the *d*–orbital electrons from the Ni_3 rings comprising Ni_3S_9 clusters to Ni_3 rings in adjacent clusters via the *p*–orbitals on the interconnecting S atoms. Vaesite, an insulator at low temperatures and a doped semiconductor at higher temperatures, lacks NiNi bond paths.