Theoretical investigation of the elastic thermodynamic, electronic and magnetic properties of $PrNi_2Si_2$ and $PrNi_2Ge_2$

Abstract

The structural, elastic, thermodynamic, electronic and magnetic properties of ferromagnetic tetragonal $PrNi_2Si_2$ and $PrNi_2Ge_2$ compounds have been calculated using the full-potential linear muffin-tin orbital (FP-LMTO) method. The exchange-correlation potential is treated within the local spin density approximation of Perdew and Wang (LSDA-PW). Moreover, we have added the Coulomb interaction U to improve the electronic band structure calculations and the magnetic properties. The calculated structural parameters are in good agreement with the experimental data. The elastic constants C_{ij} are predicted using the total energy variation versus strain technique. The polycrystalline elastic moduli, namely; shear modulus, Young's modulus, Poisson's ratio, sound velocities and Debye temperature are derived from the obtained single-crystal elastic constants. Ductility behavior of these compounds is interpreted via the calculated elastic constants C_{ij}. Electronic and bonding properties are discussed from the calculations of band structure and density of states. The thermodynamic properties are predicted through the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. The variation of the bulk modulus, lattice constant, heat capacities and Debye temperature with pressure and temperature are successfully obtained.