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First-principles investigation of mechanical and thermodynamic properties of nickel silicides at finite temperature *

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First-principles calculations are performed to investigate lattice parameters, elastic constants and 3D directional Young's modulus E of nickel silicides (i.e. β-Ni_3Si, δ-Ni_2Si, θ-Ni_2Si, ε-NiSi, and α-$NiSi_2$), and thermodynamic properties, such as the Debye temperature, heat capacity, volumetric thermal expansion coefficient, at finite temperature are also explored in combination with the quasi-harmonic Debye model. The calculated results are in a good agreement with available experimental and theoretical values. The five compounds demonstrate elastic anisotropy. The dependence on the direction of stiffness is the greatest for δ-Ni_2Si and θ-Ni_2Si, when the stress is applied, while that for β-Ni_3Si is minimal. The bulk modulus B reduces with increasing temperature, implying that the resistance to volume deformation will weaken with temperature, and the capacity gradually descend for the compound sequence of β-Ni_3Si > δ-Ni_2Si > θ-Ni_2Si > ε-NiSi > α-$NiSi_2$. The temperature dependence of the Debye temperature Θ_D is related to the change of lattice parameters, and Θ_D gradually decreases for the compound sequence of ε-NiSi > β-Ni_3Si > δ-Ni_2Si > θ-Ni_2Si > α-$NiSi_2$. The volumetric thermal expansion coefficient α_V, isochoric heat capacity C_v and isobaric heat capacity C_p of nickel silicides are proportional to T^3 at low temperature, subsequently, α_V and C_p show modest linear change at high temperature, whereas C_v obeys the Dulong-Petit limit. In addition, β-Ni_3Si has the largest capability to store or release heat at high temperature. From the perspective of solid state physics, the thermodynamic properties at finite temperature can be used to guide further experimental works and design of novel nickel-silicon alloys.

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