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Pressure dependence of elasticity in α-TiZr shape memory alloys

Abstract
Shape memory alloys are a group of materials with two noteworthy properties; shape memory effects and superelasticity thus they have attracted a number of industrial applications. Elasticity is the ability of a material to resume its normal shape after being stretched or compressed when the elastic limit is not exceeded. Titanium Nickel, copper-based and iron-based shape memory alloys are mostly applied in constructions sector but they face challenges of pressure dependency. To provide a solution, we investigated the pressure dependency of elasticity in α-TiZr shape memory alloy. Elastic constants, bulk modulus, Young modulus, shear modulus and Poisson's ratio of α-TiZr shape memory alloy were calculated at different pressure (0-10GPa) using Quantum ESPRESSO code with post-processing of the data done using Thermo_pw code. Projector augmented wave pseudo-potential with Generalized Gradient Approximations (GGA) within Perdew, Burke, and Ernzerhof (PBE) exchange-correlation functional was applied in this study. A compressive study of pressure dependency of elasticity in α-TiZr shape memory alloy is meant to avail information which may lead to adoption of this alloy in construction of intelligent reinforced concrete (IRC). Shape memory alloy wires incorporated in concrete of buildings and bridges Shape memory alloys can sense cracks and contract reducing large scale sized cracks therefore our buildings and bridges will become dynamic and sensitive to the outside changes.

Keywords

α-TiZr, Elasticity, Density functional theory

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