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Mechanical and Anisotropy Properties of SrCdPt Compound under Pressure

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ABSTRACT

The first principle calculations are performed to investigate the mechanical and anisotropy properties under the pressure of intermetallic compound SrCdPt by using density functional theory (DFT) through the PBEsol-GGA scheme. Our calculations for the elastic constants support the required stability conditions of the SrCdPt compound over the pressure range of 0 GPa to 100 GPa. The study of the shear modulus, bulk modulus, Cauchy pressure, Poisson's ratio, Pugh's ratio, and the hardness reveals that this compound is hard. Furthermore,the anisotropy properties of SrCdPt were visually illustrated and discussed by analyzing the anisotropy indexes (A1, AU, A3) and directional young's modulus, which suggesting that SrCdPt is a relatively anisotropic material and strongly pressure dependent. Additionally, the SrCdPt compound can be regarded as a candidate of incompressible and hard material. Furthermore, the Debye temperatures are also discussed by investigating the elastic constants and moduli.

1 Crystal Structure

SrCdPt crystallizes in the TiNiSi structure type. The titanium, nickel, and silicon sites are occupied by strontium, cadmium, and platinum, respectively, in thestructure of the title compound. Although platinum and nickel are in the same group in the periodic table, the platinum in SrCdPt occupies the silicon site and not the nickel site because platinum is the most electronegative metal in this structure, just like silicon in TiNiSi. The atomic structure of this compound is presented in Fig. 1

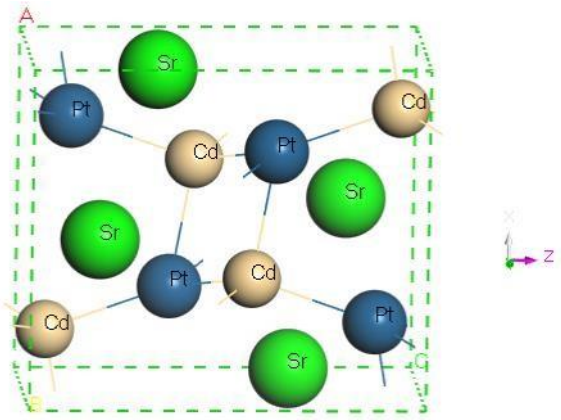

Fig. 1. Atomic structure of the intermetallic compound SrCdPt

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Results and Discussion

The elastic constants of solids provide a link between the mechanical, physical, and dynamical behavior of crystals and give important information concerning the nature of the forces operating in solids. Our results of mechanical properties under pressure are summarized in this Table as follow:

SrCdPt compound	0 GPa	100 GPa
Bulk modulus	67.146 GPa	475.844
Compressibility	0.0148	0.0021
Young modulus (GPa)	74.883 59.605 69.934	297.541 573.642 247.697
Shear modulus (GPa)		
Poisson ratio	0.298	0.392
Hardness	4.403	4.90734
Universal anisotropy index	0.359	3.551
Debye temperature (K)	212.040	363.146

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