Study of Structural and Mechanical Properties of the Half Heusler Alloy C_2CaNa

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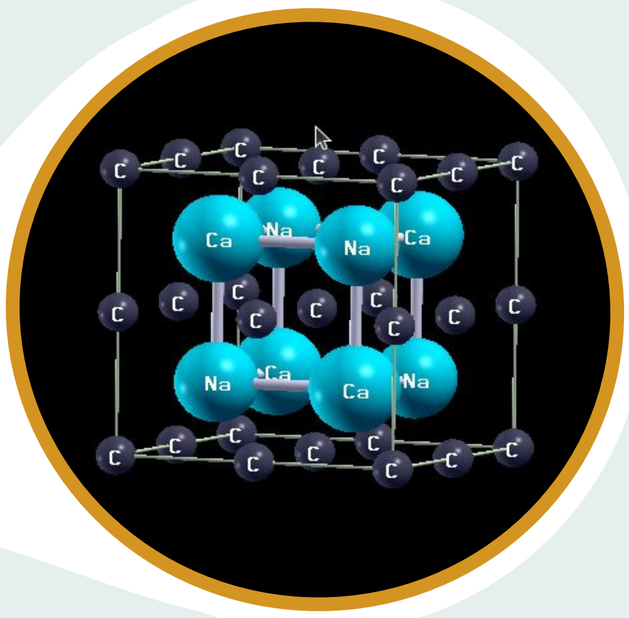
1. Introduction

Half-Heusler alloys have garnered significant attention due to their outstanding thermoelectric, magnetic, and structural properties. These materials are versatile and have the potential to revolutionize a wide range of applications, including thermoelectric generators, spintronic devices, and structural materials. Understanding the mechanical properties of these alloys is essential for their successful implementation in practical applications. In this study, we focus on the C_2CaNa (Fig. 1) half-Heusler alloy and employ density functional theory (DFT) to investigate its mechanical properties.

Fig. 1. Crystal structure (ball and stick arrangement) of the Half-Heusler C_2CaNa.



2. Methodology

In this investigation, the structural and mechanical properties of C_2CaNa half-Heusler alloy were carried out using the ab initio calculation based on DFT. The generalized gradient approximation (GGA) or hybrid functionals are suitable exchange-correlation functionals that are used in DFT calculations. The electron-ion interactions are described using the pseudopotential method, and the electronic wave functions are expanded using the plane-wave basis set. Utilizing the Quantum Espresso simulation software suite, density functional theory calculations were carried out.

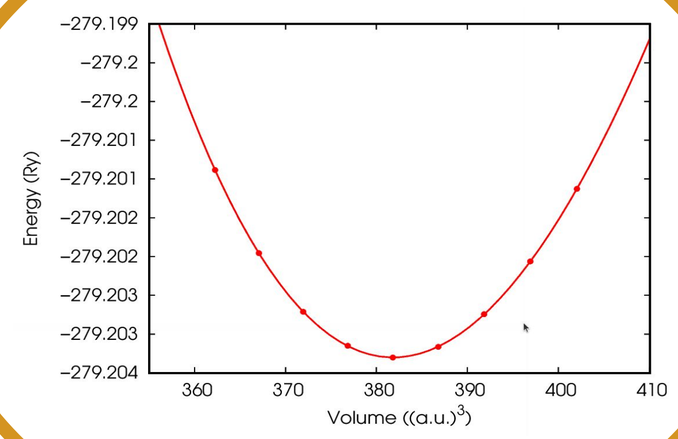
3. Results and discussion

Structural properties

We performed series of self-consistent calculations so as to optimized the structure of C_2CaNa. The data sets generated from the self-consistent total energy calculations were fitted to the fourth-order Birch–Murnaghan equation of state and the equilibrium lattice constant a_0, bulk modulus B, pressure derivative B', and band-gap E_g were obtained. The bulk modulus measures how resistant a material is to impresibility and its pressure derivative measures its response to slight increase in pressure. Fig. 2 plot of energy against volume of C_2CaNa shows that the higher the structural volume of the material the smaller the energy in respect to the bulk and pressure derivative.

From our calculated values, we observed that C_2CaNa will be easily compressed due to the small value of its bulk modulus.

Fig. 2. Plot of energy against volume for C_2CaNa.



Mechanical properties

The DFT calculations in this study revealed the following key findings: The elastic constants (Table 1.) for C_2CaNa are computed, providing insights into its mechanical stiffness and ability to resist deformation. The bulk and shear modulus values of C_2CaNa indicate the alloy's resistance to volume change and shear deformation, respectively. Young's modulus and Poisson's ratio values of C_2CaNa help characterize the material's mechanical response to different loads.

Table 1. Calculated elastic constants (C_{11}, C_{12}, and C_{44}) and Zener anisotropy factor A for C_2CaNa half-Heusler alloy

Compound	C_{11}	C_{12}	C_{44}	A, GPa
C_2CaNa	99.974	52.538	50.330	2.132

4. Conclusion

We observed that C_2CaNa will be easily compressed due to the small value of its bulk modulus. Mechanical properties revealed important insights into the elastic properties, including bulk modulus, shear modulus, Young's modulus, and Poisson's ratio. Also we determined the lattice constants and formation energies of these alloys. These findings provide valuable guidance for tailoring the mechanical properties of C_2CaNa alloys for specific applications, such as thermoelectric devices and spintronics. Overall, this study contributes to the understanding of the mechanical behavior of half-Heusler alloys and provides a foundation for further investigations and applications of C_2CaNa alloys in advanced materials.