X_2FeSi Heusler alloys: A Promising Class of Magnetic Materials

Merali Nurpeiis[1], Soltanbek Nurgul[1]
[1]Dept. of Technical physics L.N. Gumilyov Eurasian National University, Astana

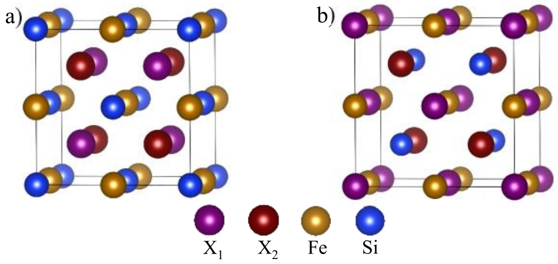
Heusler alloys, named after Fritz Heusler, are intermetallic compounds characterized by a cubic crystal structure. These alloys exhibit remarkable properties such as high spin polarization, shape memory effect, and excellent magnetocaloric properties. X_2FeSi Heusler alloys, where X represents various transition metals, have attracted particular interest due to their unique combination of magnetic and thermodynamic features.

The characteristics associated with electricity and magnetism in X_2FeSi Heusler alloys, possessing full ($L2_1$) and inverse (*XA*) crystal structures with X as Mn or V, have been investigated utilizing density functional theory (DFT). Three distinct calculation methods, namely LDA, GGA, and SCAN, were employed to examine the energy stability of the $L2_1$ and *XA* structures for these alloy compositions. The results indicate that the *XA* structure is energetically stable for both crystal structures. The choice of the functional method does not significantly influence the energy stability of the phases. Notably, the meta-GGA (SCAN) functional more accurately characterizes the electronic properties of these alloys. Through the calculations, it was determined that these compounds exhibit semimetallic behavior. An analysis from a local environment perspective was conducted to comprehend the causes behind the semimetallic band gap and the observed variations in electronic and magnetic properties in Heusler compounds. These findings align with the Slater-Pauling rule for the *XA* structure.

Crystal Structure:

X_2FeSi Heusler alloys crystallize in the face-centered cubic (*fcc*) structure, with X and Fe occupying the tetrahedral and octahedral interstitial sites, respectively, while Si atoms occupy the body-centered position. This arrangement leads to an ordered crystal structure and facilitates the manipulation of magnetic properties by adjusting the elemental composition.

Figure 1 illustrates the crystal structure of Heusler compounds, showcasing both the regular structure ($L2_1$) in Figure 1a and the inverse structure (*XA*) in Figure 1b. These structures correspond to X_2FeSi alloys, with X representing either Mn or V.



Magnetic Properties:

One of the key characteristics of X_2FeSi Heusler alloys is their tunable magnetic behavior. The presence of transition metal elements contributes to the inherent magnetism in these materials. The spin-dependent electronic structure of Heusler alloys results in high spin polarization, making them ideal candidates for spintronics applications. Moreover, X_2FeSi alloys exhibit a range of magnetic ordering, including ferromagnetic, ferrimagnetic, and antiferromagnetic, depending on the composition and atomic arrangement.

X_2FeSi Heusler alloys offer vast potential for various technological applications, including spintronics, magnetic storage devices, sensors, and energy conversion systems. Their exceptional magnetic properties, coupled with the ability to manipulate their crystal structure, make them promising candidates for next-generation electronic devices. For instance, these alloys have shown promise in spintronic devices, such as magnetic tunnel junctions, where high spin polarization is required for efficient spin injection and detection.

Despite the significant progress in understanding X_2FeSi Heusler alloys, several challenges remain. Further research is needed to optimize the alloy compositions, enhance their structural stability, and improve the reproducibility of their magnetic properties. Additionally, exploring novel synthesis techniques, such as thin film deposition and epitaxial growth, could facilitate the integration of these materials into practical devices.

X_2FeSi Heusler alloys represent a promising class of magnetic materials with tunable magnetic properties and potential applications in various fields. The ability to control their crystal structure and tailor their magnetic behavior makes them highly versatile for next-generation spintronic and magnetic storage devices. Further research and technological advancements are expected to unlock the full potential of X_2FeSi Heusler alloys and drive their integration into advanced electronic systems.

References

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Nurpeis Merali and Nurgul Soltanbek are PhD students of the Department of Technical Physics and the Department of Nanotechnology of the Eurasian National University. Their scientific interest is Heusler alloys

Nurpeiis Merali, e-mail: Nurpeis.93@mail.ru tel: +7 776 143 9900

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