# THE INFLUENCE OF PRESSURE ON THE STRUCTURAL AND ELASTIC PROPERTIES OF THE CuY INTERMETALLIC COMPOUND

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| **ABSTRACT**  Intermetallic compounds incorporating rare earth elements exhibit compelling physical and mechanical characteristics that typically surpass those of conventional metals. These properties encompass heightened strength and hardness, reduced specific gravity, enhanced corrosion resistance, and superior hot strength[1], [2]. Our investigation delved into the theoretical analysis of the intermetallic compound CuY. This study is purely theoretical, devoid of any reliance on experimental parameters. The compound adopts a cubic CsCl structure. We examined the impact of pressure on both the structural and electronic properties of the compound, employing the first principles method within the framework of Density Functional Theory (DFT). Given its significance as a crucial parameter, investigating materials under pressure holds merit. Exploring the deformation behavior of compounds subjected to compression is valuable, as it provides insights into alterations in their physical and chemical properties. Such research is indispensable for a comprehensive understanding of the nature of solids [3]. The CuY compound satisfied the Born criteria, demonstrating structurally stable properties. By utilizing elastic constants, we scrutinized the impact of increasing pressure on its mechanical properties. Furthermore, upon confirming its electronic metallic properties, we delved into the examination of the compound's response to pressure.  **References:**  [1] Gumbsch, P. and Schroll R., Atomistic aspects of the deformation of NiAl, Intermetallics, 7, 447–454, 1999.  [2] Lazar, P. and Podloucky, R., Ab initio study of the mechanical properties of NiAl microalloyed by X=Cr,Mo,Ti,Ga, Physical Review B - Condensed Matter and Materials Physics, 73, 1–8, 2006.  [3] Kars Durukan, İ., Mechanical , vibration , and optical properties of IrAl intermetallic compound via DFT calculations : high- pressure effect, Physica Scripta, 98, 075903, 2023. |

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