Mechanical and electronic properties of Al_3Zr from first-principles calculations

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Zr is used as a minor additive metal in Al alloys, and Al_3Zr formed by adding Zr to Al has $L1_2$ and $D0_{23}$ type crystal structures. Currently, there have been many studies on the recrystallization of these structures. However, comparisons based on theoretical calculations, including mechanical and thermodynamic properties and electronic structure, have not been performed well. In this study, we perform first-principles calculations on the mechanical and thermodynamic properties and electronic structure of Al_3Zr to compare the $L1_2$ and $D0_{23}$ structures of Al_3Zr on a more microscopic scale. Table 1 shows the elastic moduli and Poisson's ratios of the $L1_2$ and $D0_{23}$ structures of Al_3Zr. It can be seen that, compared to the $L1_2$ structure, the shear modulus and Young's modulus of the $D0_{23}$ structure increase, while Poisson's ratio decreases, indicating that the $D0_{23}$ structure is less ductile although its strength increases. Figure 1 shows the electronic density of states for the $L1_2$ and $D0_{23}$ structures. Compared with the $L1_2$ structure, the $D0_{23}$ structure has the Fermi energy at the center of the pseudogap. The larger this gap is, the higher the bond strength and the higher the deformation resistance, indicating that the $D0_{23}$ structure exhibits more covalent bonding than the $L1_2$ structure.

Table 1 The calculated elastic moduli (GPa), and Poisson' ratios of $L1_2$ and $D0_{23}$ structures

	B	*G*	*E*	*ν*
$L1_2$	103.47	67.11	165.53	0.233
$D0_{23}$	103.40	85.67	201.39	0.175

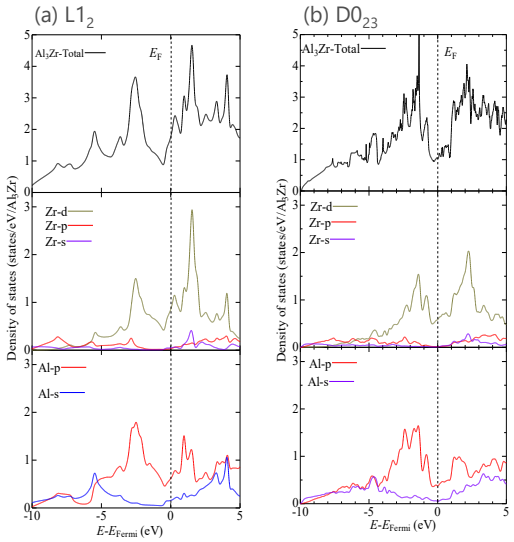

Fig. 1. Total and partial density of states for $L1_2$ and $D0_{23}$ structures. The vertial dotted lines indicate the Fermi level.