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Dislocation structure and mechanical behavior of Rh_3X $L1_2$ intermetallic alloys: combined ab-initio-Peierls-Nabarro model approach[1]
O.YU. KONTSEVOI, YU.N. GORNOSTYREV, A.J. FREEMAN, Northwestern University — Alloys based on Pt-group metals are promising materials for ultra-high temperature applications. Among them, Rh-based alloys are attractive due to a combination of high melting point, strength and superior oxidation resistance. Unfortunately, there is no information about dislocation properties and mechanisms driving their mechanical behavior. We analyzed the structure and mobility of dislocations in Rh_3X, where X = Ti, Zr, Hf, V, Nb, Ta, within the modified Peierls-Nabarro model with generalized stacking fault energetics calculated using the FLAPW method[2]. Superdislocations with type I core structure (APB-bounded) are preferred in Rh_3Ti and Rh_3Ta, whereas superdislocations with type II core (SISF-bounded) are predicted in Rh_3V and Rh_3Nb. An unusual superdislocation core structure (SISF-bounded type II′ with different sequence of Shockley partials), resulting from the unstable APB energy, was found in Rh_3Hf and Rh_3Zr. Based on our analysis of dislocation structure and mobility, we provide predictions of temperature yield stress behavior of Rh-based intermetallics, and show that their dislocation properties are closely connected with features of the electronic structure and the instability of the $L1_2$ phase with respect to $D0_{19}$ and $D0_{24}$.

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[2]Wimmer, Krakauer, Weinert, and Freeman, PRB **24**, 864 (1981)

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