Abstract Submitted
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Temperature dependence of the lattice misfit in γ/γ' superalloys: role of thermal expansion and composition changes[1] O.YU. KONTSEVOI, YU.N. GORNOSTYREV, A.J. FREEMAN, Northwestern University, K.YU. KHROMOV, Kurchatov Institute, Moscow, Russia — The magnitude of the lattice misfit δ between the γ and γ' phases is one of the key parameters determining the mechanical behavior, microstructure morphology and stability of γ/γ' high temperature superalloys. The relative importance of two contributions to the temperature dependence $\delta(T)$ are under intense investigation, namely: (i) the difference in thermal expansion of the two phases, and (ii) the redistribution of alloying component between γ and γ' with the increase of temperature. We explore the role of both contributions for the Ni-Al and Ir-Nb γ/γ' two-phase alloys based on *ab initio* full-potential total energy and phonon spectra calculations. We demonstrate that the redistribution of the major alloy components (Al into Ni and Ni into Ni_3Al) gives the main contribution to $\delta(T)$ for Ni/Ni_3Al at T >600 K. For the Ir/Ir_3Nb system, the alloy component redistribution starts to contribute to $\delta(T)$ only at extremely high temperatures (>2000 K). The amplitude of these contributions can be determined by considering the shape of the γ–γ' gap on phase diagrams. This conclusion is important for alloy design as it allows one to establish a simple relation between the alloy phase diagram and the temperature dependence $\delta(T)$.

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