Temperature dependence of the lattice misfit in $\gamma/\gamma'$ 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 $\delta$ between the $\gamma$ and $\gamma'$ phases is one of the key parameters determining the mechanical behavior, microstructure morphology and stability of $\gamma/\gamma'$ 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 $\gamma$ and $\gamma'$ with the increase of temperature. We explore the role of both contributions for the Ni-Al and Ir-Nb $\gamma/\gamma'$ 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$_3$Al) gives the main contribution to $\delta(T)$ for Ni/Ni$_3$Al at $T > 600$ K. For the Ir/Ir$_3$Nb 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 $\gamma-\gamma'$ 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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