Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Phase Stability Studies of Ni3Al and Pt3Al Structures HASANI CHAUKE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, RALF DRAUTZ, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK, BENOIT MINISINI, ISMANS, 44 Avenue Bartholdi, 72000 Le Mans, FRANCE, PHUTI NGOEPE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, DAVID PETTIFOR, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK — The structural instability of cubic L12 against the non-cubic DO'C and tP16 Pt3Al have been investigated in direct comparison with Ni3Al, using plane-wave pseudopotential methods within the local density approximation. We predict that the deleterious DO'C is more stable than cubic ductile L12 Pt3Al, in agreement with the experimental observation of the LT DO'C phase and HT L12 phase. In contrast to the Pt-Al, the L12 Ni3Al is ground state and is consistent with the experimental phase diagram. The transformation from L12 into DO'C has been investigated more explicitly, where the transformation path along DO'C leads to a stable phase at displacement parameter u=0.041?. However the Ni3Al phase, is stable at u=0.0 corresponding to the cubic L12 phase, as expected. The phonon dispersion spectra have been used to confirm the relative structural trend where a soft mode was detected for L12 and DO'C which is not found in tP16 Pt3Al.

Hasani Chauke
Materials Modeling Centre, University of Limpopo, P/Bag x1106, SOVENGA, 0727

Date submitted: 05 Dec 2007 Electronic form version 1.4