## AI-C-Ni (Aluminum-Carbon-Nickel)

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The previous work on this ternary system by [1982Sch] presented a liquidus projection and an isothermal section at 1000 °C. Recently, [2004Oht] computed three isothermal sections for this system at 1300, 1000, and 900 °C.

## **Binary Systems**

In the Al-C system [1991Har], the stoichiometric compound Al<sub>4</sub>C<sub>3</sub> ( $D7_1$ -type rhombohedral) is present. The Al-Ni phase diagram [1993Oka] shows five intermediate phases: NiAl<sub>3</sub> ( $D0_{11}$ , Fe<sub>3</sub>C-type orthorhombic), Ni<sub>2</sub>Al<sub>3</sub> ( $D5_{13}$ -type hexagonal), NiAl (B2, CsCl-type cubic, also denoted  $\beta$ ), Ni<sub>5</sub>Al<sub>3</sub> (Ga<sub>3</sub>Pt<sub>5</sub>-type orthorhombic), and Ni<sub>3</sub>Al ( $L1_2$ , AuCu<sub>3</sub>-type cubic; also denoted  $\gamma'$ ). There are no intermediate phases in the C-Ni system.

## **Computed Phase Equilibria**

In the thermodynamic modeling by [2004Oht], the regular solution approximation was applied to the liquid phase. The face-centered cubic (fcc) phase was modeled with two sublattices, one of them for the metal atoms and the other for carbon and vacancy (Va). Three sublattices were used for the body-centered cubic structure. Two metal sublattices provide for the *B*2 ordering and the third sublattice is for C and Va. The  $L1_2$  (Ni<sub>3</sub>Al) structure was described by a twosublattice model. The perovskite structure M<sub>3</sub>AlC ( $\kappa$ ) has three sublattices, with C or Va residing in the octahedral sites at the body center only of the  $L1_2$  superlattice. The formation energy of the  $\kappa$  phase was estimated from ab initio energetic calculations, using a Full Potential Linearized Augmented Plane Wave (FLAPW) method. See [2004Oht] for details.

Three isothermal sections at 1300, 1000, and 900 °C computed by [2004Oht] are shown in Fig. 1. The  $\kappa$  phase (Ni<sub>3</sub>AlC) is not stable at these temperatures. However, Ni<sub>3</sub>Al dissolves a significant amount of carbon at these temperatures.

## References

- **1982Sch:** J.C. Schuster and H. Nowotny, The Ternary System Nickel-Aluminum-Carbon, *Monatsh. Chem.*, 1982, **113**, p 163-170
- **1991Har:** K.C. Hari Kumar and V. Raghavan, A Thermodynamic Analysis of the Al-C-Fe System, *J. Phase Equilib.*, 1991, **12**(3), p 275-286
- **1993Oka:** H. Okamoto, Al-Ni (Aluminum-Nickel), J. Phase Equilib., 1993, **14**(2), p 257-259
- 2004Oht: H. Ohtani, M. Yamano, and M. Hasebe, Thermodynamic Analysis of the Co-Al-C and Ni-Al-C Systems by Incorporating Ab Initio Energetic Calculations into the CALPHAD Approach, CALPHAD, 2004, 28, p 177-190



Fig. 1 Al-C-Ni computed isothermal sections at (a) 1300, (b) 1000, and (c) 900 °C [2004Oht]