Fundamental investigation of the metastable b.c.c. phase equilibria in system Fe-Al-Ti

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In a recent work by some of the present authors [1] it was speculated that the low Mo solubility in Fe₃Al matrices can be traced back from the interaction of a metastable miscibility gap in b.c.c. Mo - Fe and the first-order A2 - B2 (FeAl) metastable equilibria in Mo concentrated compositions. This is in striking contrast with the large Ti solubility in Fe₃Al observed in the Fe-Al-Ti system, which is supposed to arise from the interaction of a stable B2 phase in the binary Ti - Fe system, which induces a continuous B2 field in the b.c.c. metastable diagram with compositions close to Fe₃AlₓTi₁−x [2]. This issue is further investigated in the present work using ab-initio calculations in the bcc Fe-Al-Ti system using the Full Potential Linear Augmented Plane Wave (FP-LAPW) electronic structure calculations in the GGA approximation combined with Cluster Variation Method (CVM) calculations in the irregular tetrahedron approximation. We also analyse the impact of the relativistic contribution on the calculated phase diagram.