Table 1: Test results of the interatomic potential for the ternary Nb-Ti-Al system developed by Farkas et. al [Modelling Simul. Mater. Sci. Eng. **4** (1996) 23-32]. The original potential files were provided by D. Farkas and converted to the LAMMPS format by Ganga Purja Pun in June 2014. This table compares cohesive energies and lattice constants of several structures computed with the original potential functions using the SOLD (Simulator of Lattice Defects) code and the converted functions using LAMMPS. The discrepancy between the two calculation methods for the $L1_2$ $NbAl_3$ phase does not reflect a conversion error but is caused by a highly wrinkled energy-volume function leading to different results depending on the initial guess and energy minimization algorithm.

Phase	Structure	Cohesive energy (eV/atom)			Lattice constant (Å)		
		SOLD	LAMMPS	Literature	SOLD	LAMMPS	Literature
Nb	BCC	7.4654242265625	7.46542422949305	7.47[1]	3.3000515328	3.30005328125001	3.3008[1]
Al	FCC	3.2063481171875	3.2063481150099	3.36[2]	3.8693398324616	3.86933749999992	4.05[2]
Ti	HCP	4.8500000625	4.8500000684133	4.85[3]	2.9510028597314[3]	2.95100018229634	2.951[3]
Nb_3Al	A15	7.30225732421875	7.30225732454802	7.22[4]	5.1260648894125	5.12606046874999	5.19[4]
$NbAl_3$	A15	4.997866328125	4.99786633061952	5.05[4]	4.9412789006898	4.94127562499995	5.14[4]
Nb_3Al	$L1_2$	6.90018734375	6.90018735080483	6.75[4]	4.054262976	4.05426164062505	4.12[4]
$NbAl_3$	$L1_2$	5.3192428125	5.3667389180349	4.86[4]	3.8375338543	3.87745565376282	4.06[4]
$TiAl_3$	$L1_2$	3.9156274609375	3.91562745013022	3.95[5]	3.960202956	3.96020312499998	4.02[5]
NbAl	B2	6.212459140625	6.21245913246315	6.27[4]	3.188834292	3.188834375	3.26[4]
NbTi	B2	6.0352174921875	6.0352174915587	5.83[4]	3.739724548	3.73972265624998	

[1] Johnson et. al, J. Mater. Res., **4** (1989) 1195.
[2] Voter et. al, MRS Symp. Proc., **82** (1987) 175.
[3] c/a = 1.588; Pasianot et. al, Phys. Rev. B, **45** (1992) 12704.
[4] Farkas et. al, Modelling Simul. Mater. Sci. Eng. **4** (1996) 23.
[5] Farkas et. al, Modelling Simul. Mater. Sci. Eng., **2** (1994) 975