Prediction of One Dimensional Long Period Structure Formation
From *Ab initio* Calculations in Al_3Ti and Cu_3Pd Compounds.

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The relative stabilities of L_{12}, $D0_{22}$, $D0_{23}$, and several one dimensional long period structures (1D-LPS) in Al_3Ti and Cu_3Pd compounds are investigated employing the Vienna ab initio simulation package (VASP). In the case of Al_3Ti compound, the energetic effects due to the tetragonal distortion of the $D0_{22}$, $D0_{23}$ structures and other 1D-LPS?s are important. The effect of the cell-internal displacements of the atoms has also been studied. After this last stage of relaxation, $D0_{23}$ is found to be the ground state. With distortion only, $D0_{22}$ is the more stable structure. 1D-LPS of the types <21j> and <2j1> have energies which are very near those of $D0_{23}$ and $D0_{22}$. In the case of Cu_3Pd compound, the energetic effects due to the tetragonal distortion and to the cell-internal displacements of the atoms are very small and the relative stabilities of the 1D-LPS studied in the present work are not modified by these relaxation effects. <3>, <4>, and <43> 1D-LPS have very similar energies of formation and are the more stable 1D-LPS?s at T=0K. In both cases, the energetic results are discussed in the framework of the axial-next-nearest-neighbor Ising (ANNNI) model.