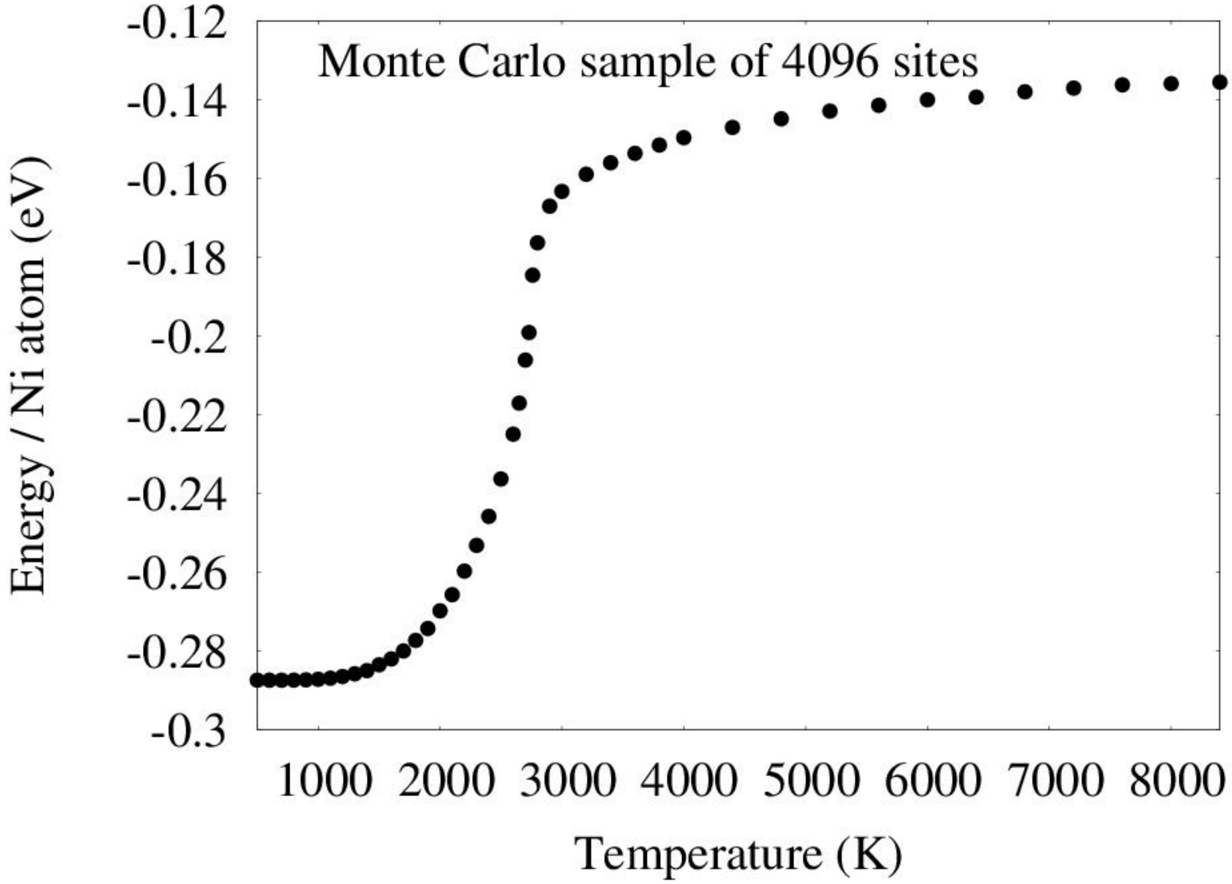

FIG. 3. Energy as function of T for the Monte Carlo runs. The phase transition happens at $T = 2750 \pm 10K$. The phase at low temperatures is certainly 353, not $L1_1$, resulting from the present choice of first-principles calculation parameters. One distinguishes the two phases by the value of $\bar{\Pi}(\sigma)$ corresponding to the nearest-neighbour tetrahedron of sites. The calculated transition temperature is much too high, even higher than the melting temperature. Two reasons concur to that: 1 - We are using an Ising Hamiltonian, not Heisenberg For instance, 2D Ising models have ordered phases, Heisenberg models have not because the transverse spin components allow paths of relaxation. 2 - We are assuming that sublattice magnetizations are unique and do not depend on spin configuration of the lattice, that is, given the concentration x the magnetization is known. Fig. 1 shows the real situation where the magnetization can fluctuate to some extent for configurations with the same x.