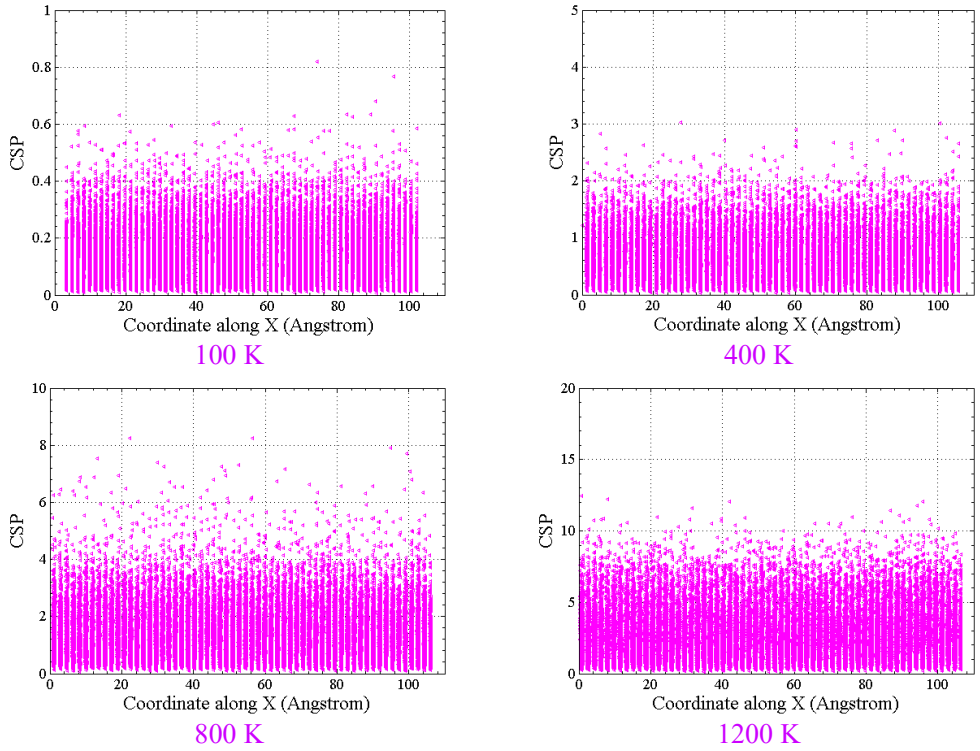

Fig. 1 Distribution of centro-symmetry parameters (CSPs) in block-shaped Ni monocrystal with an orientation of [100]-[010]-[001], heated at various temperatures. The monocrystal with periodic boundary conditions and a dimension of $30a_0$*$30a_0$*$30a_0$ (a_0, lattice constant) was energy-minimized at 0 K, prior to being heated to individual temperatures.

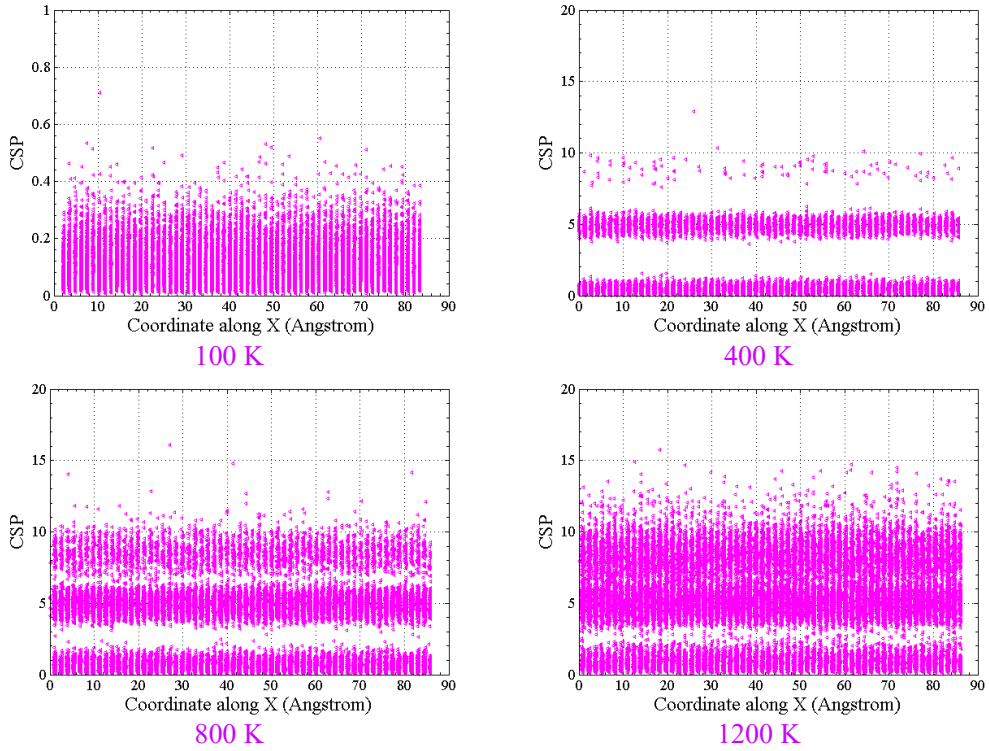

Fig. 2 Distribution of CSPs in BCC Fe monocrystal at various temperatures. The simulation settings were the same as those for Ni in Fig. 1.