MOLECULAR DYNAMICS APPROACH TO THE COMPLEX MAGNETIC STRUCTURE OF $Fe_{20}Cr_{80-x}Mn_x$ ALLOYS

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The bcc $Fe_{20}Cr_{80-x}Mn_x$ alloys have recently been reported to have the complex magnetic structure showing the spin-glass and antiferromagnetic behaviors as well as the ferromagnetic behavior, which can neither completely be determined by the neutron diffraction experiment, nor be resolved by the traditional band theory. To determine such a complex magnetic structure and to explain the magnetism, we have extended our molecular dynamics (MD) approach to the ternary alloy system, and performed the calculations using 432 atoms in the MD unit cell. Our results up to 30 at.% Mn predict the coexistence of the spin glass consisting of Fe local moments and the antiferromagnetic structure formed by Cr and Mn local moments, which can explain the low-temperature experimental data.

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