The Study of Microstructure of Large Amorphous Iron Models

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Abstract: The amorphous iron models have been constructed by the statistic relaxation method on parallel computers. We have build three models containing 5.104, 4.105 and 106 atoms. To study the influence of model size, the microstructure properties such as spherical cavities and free volume surrounding an atom have been calculated and analyzed in three models. The calculation results show that there is considerable concentration of large cavities for amorphous iron is closed to 0.024 cavities per atom.

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