Direct Microtextural Observations, and Molecular Dynamics Simulations, on the Reduction of Iron Ore.

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Abstract

After establishing, phenomologically, that reduction of industrial ore pellets depend on transformation strain and transformation induced lattice curvatures, this study was extended to direct observations on the different stages of hematite (Fe2O3) reduction. In particular, this presentation would concentrate on hematite to magnetite (Fe3O4) transformation. This appeared as an exquisite example of non-volume conserving displacive transformation, where removal of oxygen was accompanied by simple shear plus compression. Changes in lattice structures were confirmed by high resolution microtexture measurements and reactive molecular dynamic (MD) simulations.

Keywords: Reduction, Iron Ore, Microstructure, Phase transformation, EBSD, MD Simulation.

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