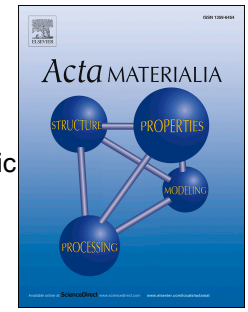
Accepted Manuscript



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PII: S1359-6454(18)30418-X

DOI: 10.1016/j.actamat.2018.05.051

Reference: AM 14604

To appear in: *Acta Materialia*

Received Date: 26 January 2018

Revised Date: 25 April 2018

Accepted Date: 23 May 2018

Please cite this article as: M. Guziewski, S.P. Coleman, C.R. Weinberger, Interface Energetics and Structure of the Pearlitic Microstructure in Steels: An Atomistic and Continuum Investigation, *Acta Materialia* (2018), doi: 10.1016/j.actamat.2018.05.051.

Interface Energetics and Structure of the Pearlitic Microstructure in Steels: An Atomistic and Continuum Investigation

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Abstract

Atomistic modeling is used to investigate the energetics and structures of commonly reported orientation relationships between ferrite and cementite within pearlite: the Bagaryatskii, the Isaichev, and the Pitsch-Petch, as well as their associated near orientations. Dislocation arrays are found to form for all orientation relationships, with their spacing and direction a function of lattice mismatch. Within each orientation relationship, different interfacial chemistries are found to produce identical dislocation spacings and line directions, but differing interfacial energies. This chemistry component to the interfacial energy is characterized and it is determined that in addition to the lattice mismatch, there are two structural factors within the cementite terminating plane that affect the energetics: the presence of like site iron pairs and proximity of carbon atoms to the interface. Additionally, an alternate method for determining the interfacial energy of systems in which there are multiple chemical potentials for a single element is developed and implemented, an approach which is likely valid for other similar systems. The Isaichev orientation relationship is found to be the most favorable, while the "near" orientation relationships are found to be at least as energetically favorable as their parent orientation relationships. A continuum model based on O-lattice theory and anisotropic continuum theory was also applied to the atomistic results, yielding interfacial energy approximations that match well with those from

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