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Impact of grain boundary structures on trapping iron

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Abstract

Density-functional theory has been used to study the segregation on iron at Σ3-(110) and Σ5-(001) twist grain boundaries. We find both grain boundaries bind interstitial iron by less than 0.4 eV, and modify the equilibrium spin state. Although interstitial Fe binds relatively weakly at fully bonded grain boundaries, it is more strongly trapped by vacancies at the grain boundary, and perhaps more critically, by Fe already trapped there. We conclude that precipitation of Fe at grain boundaries is energetically favourable, even in the absence of direct chemical bonding afforded by the substitution of Si by iron.

Key words:
`A1. Defects`, A1. Impurities, A1.Surface structure, A1. Planar defects, A1. Segregation, B3. Solar Cells
2010 MSC: 00-01, 99-00

1. Introduction

Low cost Si-based materials, including multi-crystalline silicon (mc-Si), is promising for use in photovoltaic (PV) applications [1]. mc-Si generally contains extended defects and contamination by transition elements present during module fabrication [2]. Among these elements, iron is arguably the most important detrimental impurity in lower grade Si [3], with interstitial iron (Fe_i) being

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