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Voids in silicon as a sink for interstitial iron: a density functional study

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Abstract

Transition metals, and in particular iron, are deleterious when contaminating electronic grade silicon. The gettering of these impurities to less important regions of devices is therefore a key mechanism in the optimisation of materials for applications such as photovoltaics. Voids are one potential gettering site for iron, and we present the results of a density function study on the binding of interstitial iron at such a location. We find a binding energy of around 2 eV, with the various sites at the model void lead to a wide range of binding energies. Perhaps surprisingly, we find that the most stable site lies just outside the void, which may explain the experimental observation that only a single layer of iron forms at voids. The direct relationship between binding energy and strain that caused by segregate iron atom at the sites that provided by the void structure are also presented.

Keywords: `A1. Defects`, A1. Impurities, A1.Surface structure, A1. Volume defects, A1. Segregation, B3. Solar Cells

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1. Introduction

Iron is one of the most deleterious impurities in multicrystalline silicon (mc-Si) used for solar cells [1], as interstitial iron (Fe_i) diffuses rapidly, is electrically

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