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Modelling the carbon Snoek peak in ferrite: Coupling molecular dynamics and kinetic Monte-Carlo simulations

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Abstract

Molecular statics, molecular dynamics and kinetic Monte-Carlo are used to model the carbon Snoek peak in ferrite. Using an interatomic EAM potential for the Fe–C system, saddle point energies for the diffusion of carbon have been evaluated under uniaxial stress by molecular statics. These energies have been reintroduced in a kinetic Monte-Carlo scheme to predict the repartition of carbon atoms in different octahedral sites. This repartition leads to an anelastic deformation calculated by molecular dynamics, which causes internal friction (the Snoek peak) for cyclic stress. This approach leads to quantitative predictions of the internal friction, which are in good agreement with experiments.

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1. Introduction

In body-centred cubic (bcc) metals, like α-Fe, interstitial solute atoms are found in octahedral sites, which have the characteristic to be strongly non-symmetrical, leading to local strain distortions (cubic to tetragonal symmetry). These distortions can produce anelastic relaxation observable by dynamical mechanical measurements. Snoek [1] first discovered this relaxation by measuring the internal friction of an Fe–C sample as a function of temperature. He found that the relaxation amplitude was proportional to the carbon concentration.

This proportionality has been proved for a great amount of interstitial atoms (see the insightful review of Weller [2]) and therefore is very useful to quantify precisely the amount of interstitial atoms. The position of the peak is another important information that can be deduced from internal friction analysis. It is related to interactions between interstitial atoms and the iron matrix. As these interactions contain an elastic and a chemical part, their prediction, or modelling, is far from trivial.

The linear point defect theory [2,3] has been extensively used to describe the Snoek relaxation. However, non-linear effects, such as interaction of C with interstitial solute atoms or dislocations cannot be treated properly with this theory. Some previous studies tackled this problem either analytically [4] with fitting parameters or numerically [5] with empirical pairwise interatomic potentials.

In this paper, a general scheme at the atomic scale, able to account for non-linear effects, will be presented and validated on a simple Fe–C system. A molecular statics (MS) framework based on a recently published Fe–C embedded atom method (EAM) potential [6] is used to evaluate saddle point energies as a function of external applied stress. These saddle point energies serve as entry parameters of a kinetic Monte-Carlo (KMC) simulation that describes the kinetics of carbon jumps in interstitial sites. Then molecular dynamics (MD) is used to get the anelastic

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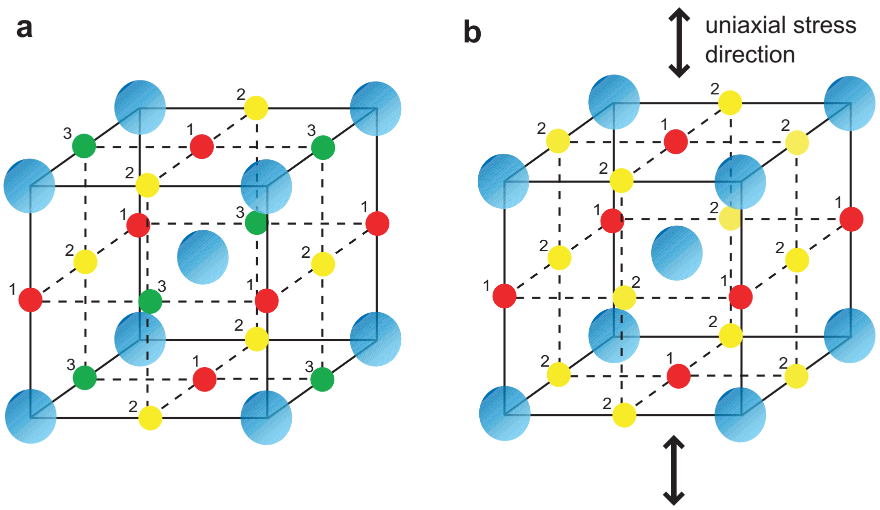

Fig. 1. (a) Three energetically equivalent octahedral sites in a stress free ferritic matrix. (b) Applying uniaxial stress leads to the formation of two energetically different octahedral sites: sites 1 (respectively 2) have their tetragonal distortion axis parallel (respectively perpendicular) to uniaxial stress direction.

distortion from the carbon population distribution (that comes out of KMC). Finally, form the applied stress and the resulting global strain, internal friction is calculated.

Some alternative approaches combined KMC with MD (*e.g.* radiation damages). In most of these works, MD results served as entry parameters for KMC [7,8]. Recent studies have tried to improve the coupling between the two methods, either by performing an “on the fly” combination of KMC and MD [9], or by extracting constitutive laws from MD calculations and incorporating them in KMC [10]. Our original scheme could be considered as a mixture of the two above mentioned techniques.

2. Snoek relaxation

Mechanical spectroscopy is a powerful experimental tool for characterising the Snoek relaxation. A cyclic stress $\sigma = \sigma_0 \cos(\omega t)$ is applied to a sample and the deformation $\epsilon = \epsilon_0 \cos(\omega t + \phi)$ is measured. The deformation can be decomposed as follows:

$$\epsilon = \epsilon'_0 \cos(\omega t) + \epsilon''_0 \sin(\omega t) \tag{1}$$

with $\epsilon'_0 = \epsilon_0 \cos(\phi)$ being the strain component in phase with stress (elastic deformation: $\sigma = \epsilon' E, E:$ Young’s modulus) and $\epsilon''_0 = \epsilon_0 \sin(\phi)$ the stain component in quadrature with stress.

The internal friction δ is defined as the ratio of the dissipated energy during one cycle (ΔW) over the maximum elastic energy (W_{el})

$$\delta = \frac{\Delta W}{W_{\text{el}}} = \frac{\int_0^{\frac{2\pi}{\omega}} \sigma \, \mathrm{d}\epsilon''}{\frac{1}{2}\sigma_0 \epsilon'_0} = 2\pi \frac{\epsilon''_0}{\epsilon'_0} = 2\pi \tan\phi \tag{2}$$

Internal friction is often referred to as $Q^{-1} = \delta/(2\pi) = \tan\phi$.

In the case of carbon in bcc iron, there are three types of octahedral sites (1, 2 and 3), which are energetically equivalent in a stress free state (Fig. 1a). Application of a uniaxial stress σ, splits the energy levels such that one site, called “site 1”[1], is different from the two others, called “site 2”[2] in the following (see Fig. 1b).

At low applied stresses (linear point defect theory), carbon jump frequency ν does not depend on stress or site types and follows an Arrhenius equation: $\nu = \nu_0 \exp[-\Delta G_0/(kT)]$, where ΔG_0 is the diffusion barrier of carbon and ν_0 the jump attempt frequency. Within the linear point defect theory [2], the system undergoes a relaxation with inverse time $\tau^{-1} = 3\nu$. Internal friction is then given by a Debye equation

$$Q^{-1} = \frac{\Delta \omega \tau}{1 + (\omega \tau)^2} \tag{3}$$

where Δ is the relaxation strength and $Q^{-1}_{\text{Max}} = \Delta/2$ is the internal friction maximum value.

To avoid the former assumption of linearity and propose a more general framework for modelling the Snoek relaxation, we need to evaluate: (i) the stress dependence of saddle point energies; (ii) the carbon distribution in each site type versus time; (iii) the anelastic deformation for a given carbon distribution. Each of these steps will be detailed in the following section.

3. Modelling internal friction: the method

3.1. Saddle point energies versus stress

To analyse the evolution of the diffusion barrier with external stress, a conjugate gradient procedure has been applied to a system of 2000 iron atoms and 1 carbon atom.

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[1] With tetragonal distortion axis parallel to uniaxial stress direction.

[2] Formerly sites 2 and 3 of Fig. 1a, with tetragonal distortion axis perpendicular to uniaxial stress direction.