

## 3-d Model for strain ordering in steel: II Relaxational effects

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**Abstract.** The spring-defect model developed by us in the accompanying paper I to discuss ferroelasticity, exhibited in the BCT phase of  $\alpha$ -iron (BCC metals), is used to analyse anelastic relaxation across the paraelastic to ferroelastic phase transition. The kinetics of the underlying Hamiltonian representing strain–strain interactions is treated within mean-field theory. The relaxation-response relation of the linear response theory is employed to derive explicit expressions for the anelastic strain, the frequency-dependent compliance and the internal friction in terms of the basic parameters of the spring-defect model.

**Keywords.**  $\alpha$ -iron; anelastic relaxation; internal friction.

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### 1. Introduction

In an earlier paper in this journal we addressed the issue of paraelastic to ferroelastic transition concomitant with BCC to BCT phase transformation in BCC metals [1] (henceforth referred to as I). In I we have argued that the BCT phase is associated with the preferential occupation of carbon atoms at one sublattice of the octahedral interstitial sites in the BCC lattice. We developed a scenario in which the presence or absence of carbon at interstitial sites in-between iron atoms was viewed to alter the interatomic distance in the iron lattice, yielding thereby a mean stretching in one direction (say  $z$ -axis) with relation to the other two mutually perpendicular directions (say the  $x$  and  $y$ -axis). This is then the main essence of our spring-defect model which is characterized by long-range Ising interactions between the carbon defects mediated by the spring forces between the host iron atoms. The structural transition from BCC to BCT phase is described by the statistical mechanics of the underlying Ising model. This theme of the spring-defect model was further expanded in I in that we derived a strain–strain interaction by associating with each carbon atom a Zener dipole [2, 3]. This allowed us to give a microscopic basis of ferroelasticity in BCC metals, and study the compliance of the system, i.e., the response to an applied stress [4, 5]. The spring-defect model provides then a natural setting for analysing dynamics.

In this paper we complement our treatment of static effects in I by investigating the corresponding dynamical effects of the BCC (paraelastic) to BCT (ferroelastic) transformation, occasioned by the hopping of carbon atoms from occupied to vacant

sites which renders the Hamiltonian time-dependent. This time-dependence (stochastic in nature) is described by the Kawasaki process of the underlying Ising model [6]. In terms of the strain variables, each Kawasaki jump, assumed to occur among the nearest neighbour sites, triggers a flip in the orientation of the principal axis of the strain tensor. This dynamics can be studied by subjecting the system to a small uniaxial stress, say along the  $z$ -axis. By relating the strain variables to carbon occupation variables we investigate the time-evolution of the macroscopic strain tensor, and in particular, its linear response to the applied stress. The latter yields the response function, and via the response-relaxation relationship, the frequency-dependent compliance [5, 4]. Our analysis is restricted to mean field theory, which is expected to provide a good approximation scheme in view of the long range nature of the strain interactions. Our work is partly motivated by recent experimental investigations which have indicated the occurrence of stress induced diffusive hopping of carbon atoms in BCC metals [7, 8].

This paper is organized in the following fashion. In §2, we introduce the kinetic equations based on the Kawasaki model. From the mean field version of these equations we develop, in §3, an analysis of the anelastic relaxation [9] as the system undergoes paraelastic (BCC) to ferroelastic (BCT) transition. Our main results on dynamics are summarized in §4.

## 2. Kinetics using mean field theory

In the case of martensitic steel, kinetic processes are governed by microscopic jumps of the carbon atoms into vacant sites induced by thermal fluctuations. The latter, while being always present even when the system is in thermal equilibrium, can lead to biased diffusion in the presence of ordering interactions. In the pseudo-spin language one imagines that the spin system described by (I.14) is in contact with a heat bath which causes spontaneous spin exchanges between two sites  $i$  and  $j$  at random instants of time. Thus, for example, a transition of the variable  $\hat{s}_i$  from the value  $+1$  to  $-1$  is accompanied by a simultaneous transition of the variable  $\hat{s}_j$  at a nearest neighbour site from the value  $-1$  to  $+1$ . This process would obviously mimic the hopping of the carbon defects from site  $i$  to site  $j$ . The appropriate master equation for the time evolution of the probability of a certain spin configuration, which specifies completely the kinetics of the problem, was written down by Kawasaki [6].

The Kawasaki process conserves the number of carbon atoms. However, a suitable combination of the sublattice magnetization which is the appropriate order parameter for the underlying 'antiferromagnetic' ordering remains nonconserved [10]. Since a rigorous treatment of such a kinetic process is quite complicated we adopt a simpler picture in which the antiferromagnetically ordered lattice is viewed as three inter-penetrating ferromagnetic lattices. This picture is easy to visualize in mean field theory in which the effective field at the  $a$  sublattice, say, is determined by three distinct interaction energies  $J_{aa}$ ,  $J_{ab}$  and  $J_{ac}$ , in addition to the local field  $h_a$  [11].

Having split the problem in terms of three sublattices it is possible to view the Kawasaki spin exchange as composite Glauber processes, one for each sublattice [12]. We may then write down for each sublattice  $a$ ,  $b$  and  $c$  the Glauber rate laws as [13]

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$$\dot{m}_a(\mathbf{r}, t) = \frac{-1}{\tau} \left[ m_a(\mathbf{r}, t) - \tanh \beta \left\{ \sum_{\mathbf{r}'} \sum_{\nu=a,b,c} J_{a\nu}(\mathbf{r} - \mathbf{r}') m_\nu(\mathbf{r}', t) + h_a(\mathbf{r}) + \mu_o \right\} \right], \quad (1)$$

$$\dot{m}_b(\mathbf{r}, t) = \frac{-1}{\tau} \left[ m_b(\mathbf{r}, t) - \tanh \beta \left\{ \sum_{\mathbf{r}'} \sum_{\nu=a,b,c} J_{b\nu}(\mathbf{r} - \mathbf{r}') m_\nu(\mathbf{r}', t) + h_b(\mathbf{r}) + \mu_o \right\} \right], \quad (2)$$

$$\dot{m}_c(\mathbf{r}, t) = \frac{-1}{\tau} \left[ m_c(\mathbf{r}, t) - \tanh \beta \left\{ \sum_{\mathbf{r}'} \sum_{\nu=a,b,c} J_{c\nu}(\mathbf{r} - \mathbf{r}') m_\nu(\mathbf{r}', t) + h_c(\mathbf{r}) + \mu_o \right\} \right], \quad (3)$$

where  $\tau$  sets the basic time scale of the Glauber process.

Assuming that we are in the 'disordered' (BCC) phase, we may linearize the above equations as

$$\dot{m}_a(\mathbf{r}, t) \simeq \frac{-1}{\tau} \left[ m_a(\mathbf{r}, t) - \beta \left\{ \sum_{\mathbf{r}'} \sum_{\nu=a,b,c} J_{a\nu}(\mathbf{r} - \mathbf{r}') m_\nu(\mathbf{r}', t) + h_a(\mathbf{r}) + \mu_o \right\} \right], \quad (4)$$

and similarly for  $m_b(\mathbf{r}, t)$  and  $m_c(\mathbf{r}, t)$ .

The Fourier transform of (4) reads

$$\dot{m}_a(\mathbf{q}, t) \simeq \frac{-1}{\tau} \left[ m_a(\mathbf{q}, t) - \beta \left\{ \sum_{\nu=a,b,c} J_{a\nu}(\mathbf{q}) m_\nu(\mathbf{q}, t) + h_a(\mathbf{q}) + \mu_o \right\} \right], \quad (5)$$

$$\dot{m}_b(\mathbf{q}, t) \simeq \frac{-1}{\tau} \left[ m_b(\mathbf{q}, t) - \beta \left\{ \sum_{\nu=a,b,c} J_{b\nu}(\mathbf{q}) m_\nu(\mathbf{q}, t) + h_b(\mathbf{q}) + \mu_o \right\} \right], \quad (6)$$

$$\dot{m}_c(\mathbf{q}, t) \simeq \frac{-1}{\tau} \left[ m_c(\mathbf{q}, t) - \beta \left\{ \sum_{\nu=a,b,c} J_{c\nu}(\mathbf{q}) m_\nu(\mathbf{q}, t) + h_c(\mathbf{q}) + \mu_o \right\} \right], \quad (7)$$

which may now be applied to study the relaxational behaviour of the system.

### 3. Anelastic relaxation

The interstitial carbon atoms in steel are centres of dilatational and deviatoric strain in the host lattice. Accordingly if a uniaxial stress is applied, it will influence the diffusive motion of atoms to the neighbouring vacant sites. This elastic diffusion, which occurs due to a gradient in the dilatation or contraction results in diffusion relaxation and anelastic strain, known as the Gorsky effect [9]. When diffusion processes take place with accompanying reorientation of the elastic dipoles over a picosecond time scale, the resultant reorientation relaxation is known as the Snoek effect, which occurs even under the presence of a homogeneous stress. In the unstressed crystal, and in the BCC phase, there is no preferential occupation of the interstitial sites, but when a uniaxial stress is applied,

the occupation of  $c$  sublattice increases, principally through nearest-neighbour jumps of atoms from  $a$  and  $b$  sublattices to the  $c$  sublattice. The result of this preferential occupation is an elongation of the crystal along the direction of the applied stress, with a matching contraction in the other two mutually perpendicular directions. Here, we investigate these effects as we approach from above the temperature  $T_s$  at which the transition from the BCC to the BCT phase takes place.

In the experimental study of anelastic relaxation one is interested in the frequency dependent compliance  $\chi(\mathbf{r}, \omega)$ . This is a measure of the strain response to an oscillatory external inhomogeneous stress. One of the powerful results of the linear response theory is that  $\chi(\mathbf{r}, \omega)$  can be obtained directly from the strain response to a time-independent stress, using the relaxation-response relation [5]:

$$\chi_{n\nu\alpha\gamma}(\mathbf{r}, \omega) = \lim_{z \rightarrow -i\omega} [z\bar{\psi}_{n\nu\alpha\gamma}(\mathbf{r}, z)], \quad (8)$$

where  $z$  is a Laplace transform variable and  $\bar{\psi}_{n\nu\alpha\gamma}(\mathbf{r}, z)$  is the Laplace transform of the so-called response function, defined by

$$\langle \hat{\epsilon}_{n\nu}(\mathbf{r}, t) \rangle = \int d\mathbf{r}' \psi_{n\nu\alpha\gamma\delta}(\mathbf{r} - \mathbf{r}', t) \sigma_{\gamma\delta}(\mathbf{r}'). \quad (9)$$

(Here we have adopted the usual convention of summation over repeated Greek indices.)

We rewrite the expression for  $\langle \hat{\epsilon}_{n\nu}(\mathbf{r}, t) \rangle$  in terms of the sublattice magnetization  $m_a$ ,  $m_b$  and  $m_c$ . Taking the Laplace transform of (5) with respect to time we have

$$zm_a(\mathbf{q}, z) - m_a(\mathbf{q}, 0) = -\frac{1}{\tau} \left[ m_a(\mathbf{q}, z) - \beta \sum_{\nu=a,b,c} J_{a\nu}(\mathbf{q}) m_\nu(\mathbf{q}, z) + \beta z^{-1} [h_a(\mathbf{q}) + \mu_0] \right], \quad (10)$$

where  $m_a(\mathbf{q}, z)$  is the Laplace transform of  $m_a(\mathbf{q}, t)$ . At time  $t = 0$  the external stress is viewed to be switched on when the system is in the BCC phase which is paramagnetic corresponding to  $\langle \hat{s} \rangle = 0$  (complete disorder). Therefore, the initial conditions are

$$m_a(\mathbf{q}, 0) = m_b(\mathbf{q}, 0) = m_c(\mathbf{q}, 0) = 0. \quad (11)$$

The stress tensor in terms of the strain tensor can be written as

$$\sigma_{n\nu}(\mathbf{q}) = L_{n\nu\alpha\gamma}(\mathbf{q}, z) \langle \hat{\epsilon}_{\alpha\gamma}(\mathbf{q}, z) \rangle, \quad (12)$$

where  $L_{n\nu\alpha\gamma}(\mathbf{q}, z)$  is the 'elastic modulus tensor'. Since the applied stress is uniaxial and along the  $z$  direction of the cubic sample,  $n = \nu = z$  and  $\alpha = \gamma = x$  or  $y$  or  $z$ , and hence we need the components of strain along  $x$ ,  $y$  and  $z$  directions only. Denoting  $L_{zzxx}(\mathbf{q}, z) = \lambda^{(1)}$ ,  $L_{zzyy}(\mathbf{q}, z) = \lambda^{(2)}$  and  $L_{zzzz}(\mathbf{q}, z) = \lambda^{(3)}$  we obtain

$$\sigma_{zz}(\mathbf{q}) = \lambda^{(1)}(\mathbf{q}, z) \langle \hat{\epsilon}_{xx}(\mathbf{q}, z) \rangle + \lambda^{(2)}(\mathbf{q}, z) \langle \hat{\epsilon}_{yy}(\mathbf{q}, z) \rangle + \lambda^{(3)}(\mathbf{q}, z) \langle \hat{\epsilon}_{zz}(\mathbf{q}, z) \rangle. \quad (13)$$

The converse relation to (12) is the one in which the strain tensor is written in terms of the stress tensor as

$$\hat{\epsilon}_{n\nu}(\mathbf{q}, z) = \psi_{n\nu\alpha\gamma}(\mathbf{q}, z) \langle \sigma_{\alpha\gamma}(\mathbf{q}) \rangle, \quad (14)$$

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where  $\psi_{n\nu\alpha\gamma}(\mathbf{q}, z)$ , the Fourier-Laplace transform of  $\psi_{n\nu\alpha\gamma}(\mathbf{r}, t)$ , is called the 'compliance tensor' with

$$\widehat{L}\widehat{\psi} = 1. \quad (15)$$

In order to obtain the expression for the modulus we first write  $m_b(\mathbf{q}, z)$  and  $m_c(\mathbf{q}, z)$  in terms of  $m_a(\mathbf{q}, z)$  as

$$\begin{aligned} m_b(\mathbf{q}, z) = & -P^{-1}(\mathbf{q}, z)[\{\beta^2 J_{bc}(\mathbf{q})J_{ca}(\mathbf{q}) + \beta J_{ba}(\mathbf{q})(1 + \tau z - \beta J_{cc}(\mathbf{q}))\}m_a(\mathbf{q}, z) \\ & + \beta z^{-1}(1 + \tau z - \beta J_{cc}(\mathbf{q}))h_b(\mathbf{q}) + z^{-1}\beta^2 J_{bc}(\mathbf{q})h_c(\mathbf{q}) \\ & - z^{-1}\beta\mu_o(1 + \tau z - \beta J_{bb}(\mathbf{q}) - \beta J_{cb}(\mathbf{q}))], \end{aligned} \quad (16)$$

and

$$\begin{aligned} m_c(\mathbf{q}, z) = & -P^{-1}(\mathbf{q}, z)[\{\beta^2 J_{ba}(\mathbf{q})J_{cb}(\mathbf{q}) + \beta J_{ca}(\mathbf{q})(1 + \tau z - \beta J_{bb}(\mathbf{q}))\}m_a(\mathbf{q}) \\ & + \beta z^{-1}(1 + \tau z - \beta J_{bb}(\mathbf{q}))h_c(\mathbf{q}) + z^{-1}\beta^2 J_{cb}(\mathbf{q})h_b(\mathbf{q}) \\ & - z^{-1}\beta\mu_o(1 + \tau z - \beta J_{cc}(\mathbf{q}) - \beta J_{bc}(\mathbf{q}))], \end{aligned} \quad (17)$$

where

$$P(\mathbf{q}, z) = [\beta^2 J_{bc}(\mathbf{q})J_{cb}(\mathbf{q}) + [1 + \tau z - \beta J_{bb}(\mathbf{q})][1 + \tau z - \beta J_{cc}(\mathbf{q})]]. \quad (18)$$

Introducing time dependence in (I.30), (I.31) and (I.32) and then taking the Laplace transform we obtain

$$m_a(\mathbf{q}, z) = \frac{a_0\Lambda^2(\mathbf{q})}{2\Delta(\mathbf{q})}H_{\mathbf{q}}I_{\mathbf{q}}[A_{\mathbf{q}}\langle\widehat{\epsilon}_{xx}(\mathbf{q}, z)\rangle + D_{\mathbf{q}}\langle\widehat{\epsilon}_{yy}(\mathbf{q}, z)\rangle + F_{\mathbf{q}}\langle\widehat{\epsilon}_{zz}(\mathbf{q}, z)\rangle], \quad (19)$$

$$m_b(\mathbf{q}, z) = \frac{a_0\Lambda^2(\mathbf{q})}{2\Delta(\mathbf{q})}G_{\mathbf{q}}I_{\mathbf{q}}[D_{\mathbf{q}}\langle\widehat{\epsilon}_{xx}(\mathbf{q}, z)\rangle + B_{\mathbf{q}}\langle\widehat{\epsilon}_{yy}(\mathbf{q}, z)\rangle + E_{\mathbf{q}}\langle\widehat{\epsilon}_{zz}(\mathbf{q}, z)\rangle], \quad (20)$$

$$m_c(\mathbf{q}, z) = \frac{a_0\Lambda^2(\mathbf{q})}{2\Delta(\mathbf{q})}G_{\mathbf{q}}H_{\mathbf{q}}[F_{\mathbf{q}}\langle\widehat{\epsilon}_{xx}(\mathbf{q}, z)\rangle + E_{\mathbf{q}}\langle\widehat{\epsilon}_{yy}(\mathbf{q}, z)\rangle + C_{\mathbf{q}}\langle\widehat{\epsilon}_{zz}(\mathbf{q}, z)\rangle]. \quad (21)$$

We now substitute the expression for  $m_b(\mathbf{q}, z)$  and  $m_c(\mathbf{q}, z)$  in  $m_a(\mathbf{q}, z)$  and using the expressions  $A_{\mathbf{q}}$  to  $I_{\mathbf{q}}$ ,  $J_{n\nu}(\mathbf{q})$ ,  $h_a(\mathbf{q})$ ,  $h_b(\mathbf{q})$ ,  $h_c(\mathbf{q})$  and equations (19)–(21), finally derive the expression for  $\sigma_{zz}(\mathbf{q})$  in terms of  $\langle\widehat{\epsilon}_{xx}\rangle$ ,  $\langle\widehat{\epsilon}_{yy}\rangle$  and  $\langle\widehat{\epsilon}_{zz}\rangle$  and all other basic microscopic parameters of the model. Comparing the expression of  $\sigma_{zz}(\mathbf{q})$  with (13) we note that the elastic moduli  $\lambda^{(1)}(\mathbf{q}, z)$ ,  $\lambda^{(2)}(\mathbf{q}, z)$  and  $\lambda^{(3)}(\mathbf{q}, z)$  take the form

$$\begin{aligned} \lambda^{(1)}(\mathbf{q}, z) = & \frac{za_0^2\Lambda^2(\mathbf{q})H_{\mathbf{q}}I_{\mathbf{q}}A_{\mathbf{q}}}{4\beta V\Delta(\mathbf{q})G_{\mathbf{q}}(D_{\mathbf{q}}E_{\mathbf{q}} - B_{\mathbf{q}}F_{\mathbf{q}})}[\Lambda(\mathbf{q})(1 + \tau z) \\ & - \beta\{G_{\mathbf{q}}^2[B_{\mathbf{q}}C_{\mathbf{q}} - E_{\mathbf{q}}^2] + H_{\mathbf{q}}^2[A_{\mathbf{q}}C_{\mathbf{q}} - F_{\mathbf{q}}^2] \\ & + I_{\mathbf{q}}^2[A_{\mathbf{q}}B_{\mathbf{q}} - D_{\mathbf{q}}^2]\} - \text{higher order in } \beta], \end{aligned} \quad (22)$$

with  $\lambda^{(2)}(\mathbf{q}, z)$  and  $\lambda^{(3)}(\mathbf{q}, z)$  obtained from (22) by replacing  $A_{\mathbf{q}}$  by  $D_{\mathbf{q}}$  and  $F_{\mathbf{q}}$  respectively in the overall prefactor of the numerator. Inverting the expressions for  $\lambda^{(1)}(\mathbf{q}, z)$ ,  $\lambda^{(2)}(\mathbf{q}, z)$  and  $\lambda^{(3)}(\mathbf{q}, z)$  we get the corresponding expressions for the response function  $\psi^{(1)}(\mathbf{q}, z)$ ,  $\psi^{(2)}(\mathbf{q}, z)$  and  $\psi^{(3)}(\mathbf{q}, z)$  respectively, where  $\tilde{\psi}_{zzxx}(\mathbf{q}, z) = \psi^{(1)}(\mathbf{q}, z)$ ,

$\tilde{\psi}_{zzyy}(\mathbf{q}, z) = \psi^{(2)}(\mathbf{q}, z)$  and  $\tilde{\psi}_{zzzz}(\mathbf{q}, z) = \psi^{(3)}(\mathbf{q}, z)$ . Thus

$$\begin{aligned} \psi^{(3)}(\mathbf{q}, z) = & \frac{4\beta V \Delta(\mathbf{q}) G_{\mathbf{q}} (D_{\mathbf{q}} E_{\mathbf{q}} - B_{\mathbf{q}} F_{\mathbf{q}})}{z a_o^2 \Lambda^2(\mathbf{q}) H_{\mathbf{q}} I_{\mathbf{q}} F_{\mathbf{q}}} [\Lambda(\mathbf{q})(1 + \tau z)] \\ & - \beta \{ G_{\mathbf{q}}^2 [B_{\mathbf{q}} C_{\mathbf{q}} - E_{\mathbf{q}}^2] + H_{\mathbf{q}}^2 [A_{\mathbf{q}} C_{\mathbf{q}} - F_{\mathbf{q}}^2] \\ & + I_{\mathbf{q}}^2 [A_{\mathbf{q}} B_{\mathbf{q}} - D_{\mathbf{q}}^2] \} - \text{higher order in } \beta^{-1}, \end{aligned} \quad (23)$$

with  $\psi^{(1)}(\mathbf{q}, z)$  obtained from (22) by inverting the expression for  $\lambda^{(1)}(\mathbf{q}, z)$ . The expression for the frequency dependent compliance is obtained from (23) (by neglecting terms of order  $\beta^2$ ) and then using (8), when the transition temperature is approached from the disordered BCC phase. Thus

$$\chi^{(3)}(\mathbf{q}, \omega) \simeq \frac{4\beta V \Delta(\mathbf{q}) G_{\mathbf{q}} (D_{\mathbf{q}} E_{\mathbf{q}} - B_{\mathbf{q}} F_{\mathbf{q}})}{a_o^2 \Lambda^3(\mathbf{q}) H_{\mathbf{q}} I_{\mathbf{q}} F_{\mathbf{q}}} \frac{1}{[1 - \frac{1}{4} \beta J(\mathbf{q})][1 - i\omega\tau_{\mathbf{q}}]}, \quad (24)$$

where the relaxation time  $\tau_{\mathbf{q}}$  and the interaction  $J(\mathbf{q})$  are defined as

$$\tau_{\mathbf{q}} = \tau \left[ 1 - \frac{1}{4} \beta J(\mathbf{q}) \right]^{-1}, \quad (25)$$

$$J(\mathbf{q}) = \frac{4}{\Lambda(\mathbf{q})} \{ G_{\mathbf{q}}^2 [B_{\mathbf{q}} C_{\mathbf{q}} - E_{\mathbf{q}}^2] + H_{\mathbf{q}}^2 [A_{\mathbf{q}} C_{\mathbf{q}} - F_{\mathbf{q}}^2] + I_{\mathbf{q}}^2 [A_{\mathbf{q}} B_{\mathbf{q}} - D_{\mathbf{q}}^2] \}. \quad (26)$$

Therefore the relaxation time associated with every  $\mathbf{q}$  mode diverges when the following condition is satisfied:

$$\frac{1}{4} \beta J(\mathbf{q}) = 1. \quad (27)$$

As discussed in I (§ 4.2), a by-product of (24) is an expression for the transition temperature  $T_s$  as given in (I.78). Expanding the expressions from  $A_{\mathbf{q}}$  to  $I_{\mathbf{q}}$  for small  $\mathbf{q}$  we obtain

$$T_s \simeq \frac{4\alpha^2 K'^3 [4K + 3K']}{k_B [K^2 (K + 6K') + 8K'^2 (K + 2K')]}, \quad (28)$$

which is the ferroelastic transition temperature at which the internal friction (to an applied inhomogeneous stress) diverges. Note that  $T_s$  is completely determined by the basic parameters of the spring-defect model.

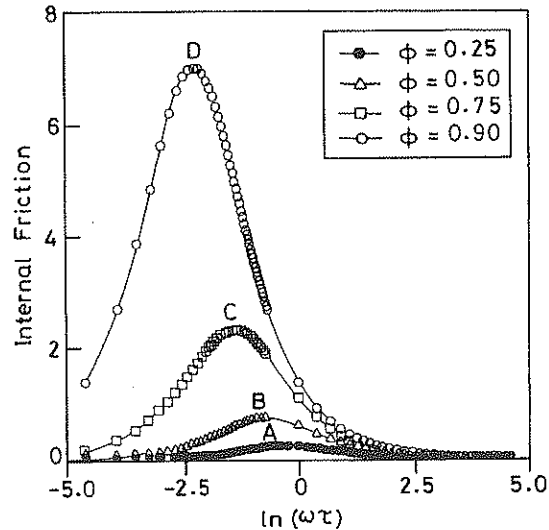
The internal friction or the loss tangent can now be readily obtained from (24) using the relation

$$\tan \phi(\omega) = \chi_u^{-1} \Im \chi(0, \omega), \quad (29)$$

(where  $\Im$  stands for the imaginary part)

$$\Im \chi^{(3)}(\mathbf{q}, \omega) = \frac{4\beta V \Delta(\mathbf{q}) G_{\mathbf{q}} (D_{\mathbf{q}} E_{\mathbf{q}} - B_{\mathbf{q}} F_{\mathbf{q}})}{a_o^2 \Lambda^3(\mathbf{q}) H_{\mathbf{q}} I_{\mathbf{q}} F_{\mathbf{q}}} \frac{1}{[1 - \frac{1}{4} \beta J(\mathbf{q})]} \frac{\omega \tau_{\mathbf{q}}}{[1 + \omega^2 \tau_{\mathbf{q}}^2]}, \quad (30)$$

where  $\chi_u$  is the (unrelaxed) elastic modulus of the host material. Numerical results for the internal friction are presented in figure 1. In the high temperature limit (disordered BCC



**Figure 1.** The internal friction, versus  $\ln(\omega\tau)$ , for different values of  $\phi = T_s/T$ . Curve A,  $\phi = 0.25$ ; curve B,  $\phi = 0.5$ ; curve C,  $\phi = 0.75$  and curve D,  $\phi = 0.9$ . It can be seen that as  $T$  approaches the phase transformation point ( $T_s$ ) (i.e. as  $\phi$  increases), the internal friction peak exhibits a shift and a broadening.

phase) and for  $\omega = 0$  (static case) the above expression (24) reduces to the expected Curie form as given by (I.76). The expected Curie–Weiss form of the static compliance is recovered from (24) (by neglecting terms of order  $\beta^2$ ) when the transition temperature is approached from the BCC phase. This has already been given in (I.77). The Curie–Weiss law for the static compliance as well as the frequency dependent compliance, as the system develops a spontaneous strain while undergoing a transition from the high temperature BCC phase to the low temperature BCT phase, is similar to the one derived by Dattagupta *et al*, in a different model [4].

#### 4. Results

Our principal aim in this paper was to study the diffusive behaviour of the interacting interstitial carbon defects in BCC metals and the associated anelastic relaxation [14]. The question of kinetics is of great importance, especially in relation to the hopping diffusion of carbon in steel. As the carbon jumps into the neighbouring site the associated Zener dipole flips its orientation, leading to anelastic relaxation [2, 3, 9]. At the microscopic level each flip of the Zener dipole is linked with an exchange of sites by a carbon–vacancy pair, which in the Ising language, can be described by a Kawasaki process [6]. Thus all relaxational characteristics associated with frequency-dependent compliance, internal friction, etc., can be studied by means of the Kawasaki model. We have used mean field approach (MFA) which is based on Glauber spin flip in each sublattices. The internal friction is derived in terms of basic parameters of an underlying spring–defect model such as  $K$ ,  $K'$  and  $\alpha$ . The internal friction peak based on (29) is plotted for different  $T_s/T$ . The

four curves in figure 1 correspond to four different values of  $T_s/T$ . We observe that as  $T_s/T$  increases, the peak position shifts towards  $\omega\tau \ll 1$  region, i.e. towards higher temperature, if we assume an Arrhenius form for  $\tau$ . The shift is accompanied by a broadening and an increase in height of the peak. These features are in qualitative agreement with the experimental finding of Weller *et al* in the Ta–O system [15]. The plot of internal friction has been shown to exhibit a shift and a broadening of the peak as the transition temperature is approached from above in the BCC phase.

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