Exact analytical solution of the internal friction associated with a geometric kink chain oscillating in an atmosphere of paraelastic interstitials and decorated by a dragging point defect

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The partial differential equation which describes the geometric kink chain oscillating in an atmosphere of uniformly distributed paraelastic interstitials and, in addition, decorated by a dragging point defect at the midpoint, is solved exactly with use of the Laplace-transformation technique. The internal friction coefficient and the modulus defect are obtained in closed forms which indicate the existence of two separate peaks. The Cole-Cole diagrams are also investigated which show irrevocably the splitting of the original cold-work peak into two subpeaks with an increase of the drag strength of the decorating point defect.

I. INTRODUCTION

The foremost theoretical description of dislocation damping was formulated by Koehler[1] and later developed in more detail by Granato and Lücke.[2,3] In the standard theory, dislocations are treated as the analog of strings and the damping is determined by the viscosity of the lattice and the length of such strings. In the Koehler-Granato-Lücke (KGL) theory not only the nodal points on the dislocation network, which are intrinsic pinners, but also the point defects which lie on dislocations are taken as firm pinning points. The work of Simpson, Sosin, and Johnson[4,5] on electron-irradiated copper and the study of Seiffert, Simpson, and Sosin[6] and Seiffert[7] on electron-irradiated high-purity polycrystalline aluminum suggest that the standard KGL theory should be generalized to allow the point defects to be dragged with the oscillating dislocation line. For many years, experiments on internal friction were interpreted in terms of the early dragging-point-defect theory of Schoeck[8] or Simpson and Sosin[9] where the inertial term, which is especially important at high frequencies, was completely neglected in their treatment.

In the view of certain inconsistencies as discussed by Hirth[10] in great detail, Seeger,[11] for the general case of interstitials (C,N,O,H) in body-centered-cubic metals (bcc), and Hirth,[12] for the specific case of interstitial hydrogen in bcc iron, suggested that the cold-work peak could be explained instead by a kink-pair model. Another possible source for the cold-work peak formation is the harmonic oscillations of the geometric kink chain in the atmosphere of paraelastic interstitials as discussed extensively by Ogurtani and Seeger[13,14] in recent years.

We should mention here very clearly that the geometric kink-chain model, which was utilized by Seeger and Schiller,[15] Suzuki and Elbaum,[16] and later by Ogurtani and Seeger,[13,14] has an identical mathematical macrostructure in comparison with the dislocation-string model (in linear dissipative mode), which was advocated by Koehler,[1] and extensively employed by Granato and Lücke,[17,18] Schoeck,[8] Simpson and Sosin,[9,19] Brailsford,[20] and later by Ogurtani[21] in dislocation relaxation phenomena in metals that were subjected to severe plastic deformation, as long as one stays in the domain of the linear Newtonian viscosity regime.[22,23]

In the present paper, in order to elucidate the importance of the decoration of the geometric kinks along the nonscrew dislocations in bcc metals by heavy dragging interstitials, in a highly localized fashion, the complete mathematical analysis of a partial differential equation will be given in terms of a Laplace-transformation technique. This partial differential equation contains not only a linear and uniform drag-force term associated with the atmosphere of paraelastic interstitials but also a localized power dissipation contribution due to additional point defects (may be the same type of interstitial species) at the midpoint of the kink chain or dislocation string.[18] Using the compact or closed form of the exact solution, which is for the first time obtained by the author, the internal friction coefficient and the modulus defect are calculated in Sec. III. The general behavior of the internal friction coefficient as well as the Cole-Cole diagrams are simulated using the plotter facilities of an IBM-PC60 minicomputer by the newly introduced normalization technique of Sec. IV.

II. KINK-CHAIN DYNAMICS UNDER THE ACTION OF A LOCALIZED DRAGGING-POINT-DEFECT DECORATION

According to our extensive analysis as well as computer modeling experiments[13,14] the mathematical model for the equation of motion of a geometric kink chain which is decorated by a mobile (dragging) point defect at the midposition may be given by the following partial differential equation:

$$M_k \partial_{tt}^2 u + [B_0 + B_d \delta(x - L/2)]\partial_t u - c_k \partial_{xx}^2 u = F_k \sin(\omega t), \tag{1}$$

where $c_k = S_0^{\mathrm{el}}(a_k^2/2d_k)$ and $F_k = ba_k\sigma_r$. Here, S_0^{el} is the logarithmic factor of the elastic part of the dislocation line tension, d_k is the equilibrium separation between the kinks along the dislocation line, B_0 is the drag coefficient associated with the uniformly distributed interstitial cloud, and B_d is the damping constant of the decorating point defect. Similarly, M_k is the effective mass of a kink, a_k the spacing between neighboring Peierls valleys, b is the Burgers vector, and σ_r is the resolved shear stress.

As a typical application of the Laplace transform, the following expression is obtained from Eq. (1) plus the boundary conditions of the initial rest state:

$$M_k p^2 \bar{u} + p[B_0 + B_d \delta(x - L/2)]\bar{u} - c_k \frac{d^2\bar{u}}{dx^2} = F_k/(p - i\omega) \; ; \quad (2)$$

similarly, the natural boundary conditions become

$$\bar{u}(0) = \bar{u}(L) = 0 \; . \quad (3)$$

The overbar on any function denotes the Laplace transform of that function. The above boundary-value problem has the following exact solution in the Laplace space:

$$\bar{u}_I(x) = 2\bar{u}_p \sinh(\beta x/2) \frac{\sinh[\beta(L-x)/2] + (2pd_1/\beta\omega_0)\sinh(\beta L/4)\sinh[\beta(L/2-x)/2]}{\cosh(\beta L/2) + (pd_1/\beta\omega_0)\sinh(\beta L/2)} , \quad 0 \le x < L/2 \quad (4)$$

where we have used the following substitutions: $d_0 = B_0/M_k$, $d_1 = B_d/M_k$, $\omega_0^2 = c_k/M_k$ (the natural frequency of the system), and $\beta^2 = p(p + d_0)/\omega_0^2$. Here, u_p represents the particular solution of the differential equation (3), and it is given by $\bar{u}_p = (F_k/M_k)/p(p+d_0)(p - i\omega)$. The solution in the region of $L/2 < x \le L$ is the mirror image of $\bar{u}_I(x)$ with respect to $x = L/2$.

For the internal friction phenomena we are interested in the steady-state solution of the problem that can be immediately obtained from Eq. (4) by the inverse Laplace-transformation procedure, which yields

$$u_I(x,t) = 2\sinh(Ax/2\omega_0) \frac{A\sinh[A(L-x)2\omega_0] + (2id_1\omega/\omega_0)\sinh(AL/4\omega_0)\sinh[A(L-2x)/4]}{A\cosh(AL/2\omega_0) + (id_1\omega/\omega_0)\sinh(AL/2\omega_0)} \times (F_k/M_k A^2)\exp(i\omega t) \; , \quad (5)$$

where $A = [i(i + d_0)]^{1/2}$, and the imaginary part of the above expression is the one that corresponds to the solution (steady state) of Eq. (1). The correctness of this expression can be easily verified if one takes $d_1 \to \infty$, then one has, from Eq. (5),

$$u_I(x,t) \to 2\sinh(Ax/2\omega_0) \frac{\sinh[A(L-2x)/4\omega_0]}{\cosh(AL/4\omega_0)} \times (F_k/M_k A^2)\exp(i\omega t) \; , \quad (6)$$

which shows that the loop length became $L/2$, and the dragging[13] point defect became the "firm pinning point."

III. THE DECREMENT AND THE MODULUS DEFECT

To find the decrement and the apparent modulus change we will follow the general procedures of Nowick,[24] with the exception of the internal friction directly associated with the isolated dragging-point-defect motion (singularity), where we will utilize the more general concept of energy dissipation in the calculation of the internal friction contribution directly related to the dragging-point-defect motion itself. Actually, we have done a thorough treatment of this problem by utilizing three different procedures: the calculation of the energy loss directly from the drag-force term, the calculation of the total energy loss from the power-input term, and finally the limited Nowick procedure, as described in this paper. All seemingly independent procedures resulted in exactly the same answer.

The dislocation strain ϵ_d produced by a loop of length L in a cube of unit dimensions is usually given by $Lb\langle u \rangle$, where $\langle u \rangle$ is the average displacement of a dislocation of length L. Thus, if Λ is the total length (the density of dislocations) of the movable dislocation line,

$$\epsilon_d = \Lambda b(2/L)\int_0^{L/2} u_I(x,t)dx \; , \quad (7)$$

due to the symmetry with respect to the midpoint at which the isolated dragging-point defect is situated. The relation between the total strain ϵ_t and the applied stress can be written

$$\epsilon_t = J^{\dagger}(\omega)\sigma_r \exp(i\omega t) \; , \quad (8)$$

where $\epsilon_t = \epsilon_e + \epsilon_d$. The elastic strain ϵ_e is given by the elasticity theory, $\epsilon_e = \sigma_r \exp(i\omega t)/G$. With these definitions of stress and strain, the appropriate measure of the internal friction is the logarithmic decrement

$$\delta = \pi J_2(\omega)/J_1(\omega) \cong \pi G J_2^d(\omega) \; , \quad (9)$$

where $J(\omega) = J_1(\omega) + iJ_2(\omega)$. Similarly, the modulus defect (the apparent fractional decrease in elastic modulus due to dislocation motion)

$$\Delta G/G = GJ_1(\omega) - 1 \cong GJ_1^d(\omega) \ . \tag{10}$$

In the calculation of the average displacement of a dislocation loop of length L, we will intentionally use the closed form which is given by Eq. (5). However, first let us introduce the parameter α as

$$\alpha^2 = i\omega(i\omega + d_0)/\omega_0^2 \ , \tag{11}$$

which upon substitution in Eq. (5) yields, with the usage in the integration as denoted by Eq. (7),

$$\epsilon_d = \frac{2\Lambda b^2 \sigma_r e^{i\omega t}}{C_k \alpha^3 L} \left[\alpha L/2 - \frac{\sinh(\alpha L/2) + 4i(\mu_d^2/\alpha L)\sinh^2(\alpha L/4)}{\cosh(\alpha L/2) + i(\mu_d^2/\alpha L)\sinh(\alpha L/2)} \right] , \tag{12}$$

where $\mu_d^2 = \omega B_d L/2C_k$. On the other hand, it is very useful to introduce the identity[13] that can be obtained from Eq. (11),

$$\alpha = (\mu_0 M_0/L)\exp(i\theta_0) \ , \tag{13}$$

where

$$M_0^2 = 2(1 + \omega^2 M_k^2/B_0^2)^{1/2} \ , \tag{14}$$

$$2\theta_0 = \tan^{-1}(B_0/M_k\omega) \ , \tag{15}$$

and

$$\mu_0^2 = \omega B_0 L^2/2C_k \ . \tag{16}$$

Here, the latter parameter μ_0 is a dimensionless parameter which was also introduced by Simpson and Sosin[9] and Ogurtani.[13] Now and then we are going to restrict our treatment of the problem for the relaxation mode, where the inertial term M_k is taken to be equal to zero, which results in $M_0 = 2^{1/2}$ and $\theta = \pi/4$ from Eqs. (14) and (15). Upon substituting these results into Eqs. (13) and (12), one can obtain the following exact expressions for the logarithmic decrement and the modulus defect, after very tedious mathematical manipulations (the observed spectrum):

$$\begin{aligned}\delta_T = \delta_0 \Lambda L^2(\pi^4/16\mu_0^3)[\mu_0 - (\,&(\sinh\mu_0 + \sin\mu_0)/2 + R\mu_0[\cosh\mu_0 + \cos\mu_0 - 2\cosh(\mu_0/2)\cos(\mu_0/2)] \\ &+ R^2(\mu_0^2/2)\{\sinh\mu_0 - \sin\mu_0 + 2[\cosh(\mu_0/2)\sin(\mu_0/2) - \sinh(\mu_0/2)\cos(\mu_0/2)]\}\,)/D\] \ ,\end{aligned} \tag{17}$$

and

$$\begin{aligned}\Delta G/G = \delta_0 \Lambda L^2(\pi^3/16\mu_0^3)(\,&(\sinh\mu_0 - \sin\mu_0)/2 + R\mu_0[\cosh\mu_0 - \cos\mu_0 - 4\sinh(\mu_0/2)\sin(\mu_0/2)]/2 \\ &+ R^2(\mu_0^2/2)\{\sinh\mu_0 + \sin\mu_0 - 2[\sinh(\mu_0/2)\cos(\mu_0/2) + \cosh(\mu_0/2)\sin(\mu_0/2)]\}\,)/D \ ,\end{aligned} \tag{18}$$

where

$$\begin{aligned}D = &(\cosh\mu_0 + \cos\mu_0)/2 + R\mu_0(\sinh\mu_0 - \sin\mu_0)/2 \\ &+ R^2\mu_0^2(\cosh\mu_0 - \cos\mu_0)/4 \ .\end{aligned} \tag{19}$$

In the above expressions we utilized the following short hand notations: $R = (\mu_d/\mu_0)^2$, and $\delta_0 = 8Gb^2/\pi^3 C_k$, where R is a very important system parameter which is also equal to B_d/LB_0.

Up to now we have been dealing with the energy dissipation, which is continuously distributed along the kink chain taking into account the localized (singularity) dissipation at the point-defect decoration. One can easily show that the energy dissipation per cycle at the point-defect decorator may be given by

$$\Delta W_{\text{deco}} = (\pi B_d/\omega)\partial_t u_I(L/2,t)\partial_t u_I^\dagger(L/2,t) \ , \tag{20}$$

and the total energy loss due to point-defect decorators per unit volume of the sample may be written as $\Delta W_{\text{deco}}^T = (\Lambda/L)\Delta W_{\text{deco}}$. Hence the associated logarithmic decrement for the point-defect decorators can have the following expression by utilizing Eq. (5) properly in the relaxation mode ($M_k \to 0$):

$$\delta_{\text{deco}} = \delta_0 \Lambda L^2(\pi^4/16\mu_0^3)R\mu_0[\cosh(\mu_0/2) - \cos(\mu_0/2)]/D \ , \tag{21}$$

where we first made the calculation of the internal friction coefficient $Q^{-1} = \Delta W_{\text{deco}}^T/(\pi\sigma_r^2/G)$, then used the approximate relationship between the logarithmic decrement and the internal friction coefficient, $\delta \cong \pi Q^{-1}$.

IV. DISCUSSION

In order to illustrate the general behavior of the decrement which is usually measured at a given driving frequency as a function of temperature, we have decided to introduce a new universal plotting procedure in Fig. 1, where the logarithmic decrements obtained from Eqs.

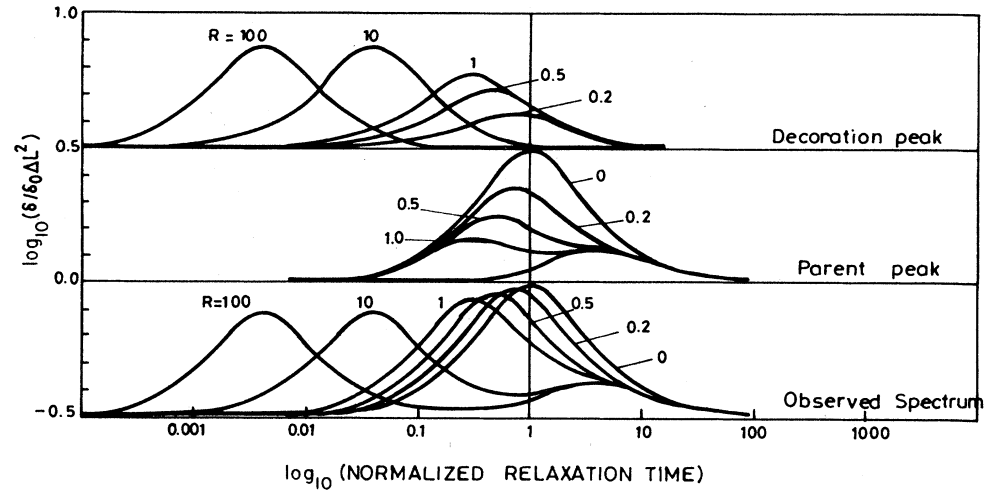

FIG. 1. Decrement plotted as a function of the renormalized frequency $\Omega_{B_0}=\omega/\omega_{B_0}^0$ for various values of the damping strength ratio R. The observed peaks are obtained according to Eq. (17), and the decoration peaks are calculated using Eq. (21). The difference between these two peaks yields the relaxation peak associated with the uniformly distributed paraelastic interstitials called the parent peak.

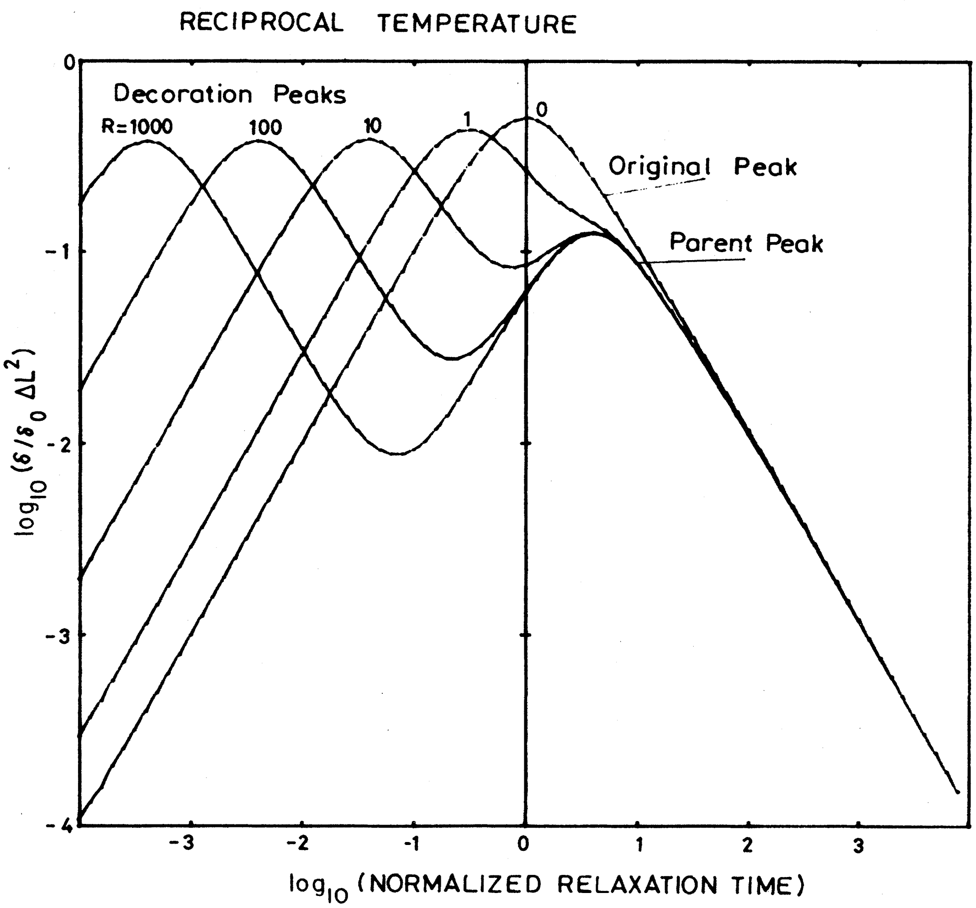

FIG. 2. The observed peaks are given as a function of the renormalized relaxation frequency on a double-logarithmic plot for various values of the damping strength ratio. The decomposition of the observed peak into two Debye-type relaxation peaks, the decoration peak and the parent peak, for large values of R is clearly illustrated in these plots.

(17) and (21) are shown with respect to the renormalized relaxation time $\Omega_{B_0}=\omega/\omega_{B_0}^0$ for the various values of the damping strength ratio R. Here, by definition, we have $\mu_0^2=(\pi^2/2)\Omega_{B_0}$, which was also utilized by the author in his previous work.[13] $\omega_{B_0}^0$ is really the fundamental relaxation frequency of a vibrating kink chain without inertia, and it is given by $\omega_{B_0}^0=(\pi/L)^2C_k/B_0$. In this plot the peak which is denoted as the parent peak is associated with the uniformly distributed interstitials along the kink chain, and it is obtained by the following relationship: $\delta_P=\delta_T-\delta_{\text{deco}}$. Figure 1 reveals that, when $R=0$, which corresponds to the case without the decorating point defect, the increment δ_T indicates a well-defined single maximum with respect to the viscous drag coefficient B_0, or the temperature, at $\Omega_{B_0}=1$. Similarly, for the large values of the damping strength ratio, namely, $R>10$, the complete separation of the observed internal friction coefficient δ_T takes place, where at the low-temperature side (the large values of Ω_{B_0}) the parent peak due to paraelastic interstitials is situated, and at the high-temperature side (the low values of Ω_{B_0}) a new peak which is directly related to the localized point-defect decoration is placed. As can be seen from Fig. 2, both peaks, the decoration peak and the parent peak, are exactly Debye type in shape. For this terminal regime, the parent peak has a relaxation strength which is a factor of 4 smaller than the original peak without the decorator. Also, there is a proper peak shift in the parent relaxation peak according to the new loop length of $L/2$. Therefore, as one might expect, intuitively, the sticky heavy decorator becomes a firm pinning point as far as the relaxation behavior of the kink chain is concerned.

The true nature of the decoration peak which is calculated according to Eq. (21) can be easily understood if one investigates the limiting behavior, analytically. Namely, one can obtain the following expression for large values of R and small values of μ_0 by keeping $\mu_d^2=R\mu_0^2$ constant during the limit procedure:

$$\delta_{\text{deco}}\rightarrow\delta_0\Lambda L^2(\pi^4/128)(\mu_d^2/2)/(1+\mu_d^4/4)\ , \tag{22}$$

or equally well one has the following form:

$$\delta_{\text{deco}}\rightarrow\delta_0\Lambda L^2(\pi^4/128)(\pi^2\Omega_d/4)/[1+(\pi^2\Omega_d/4)^2]\ , \tag{23}$$

where $\Omega_d=\omega B_dL/\pi^2C_k$ is the normalized relaxation time of the decorator. The expression (23) represents the logarithmic decrement of the kink chain which is dragged by an isolated point defect at the middle, and in

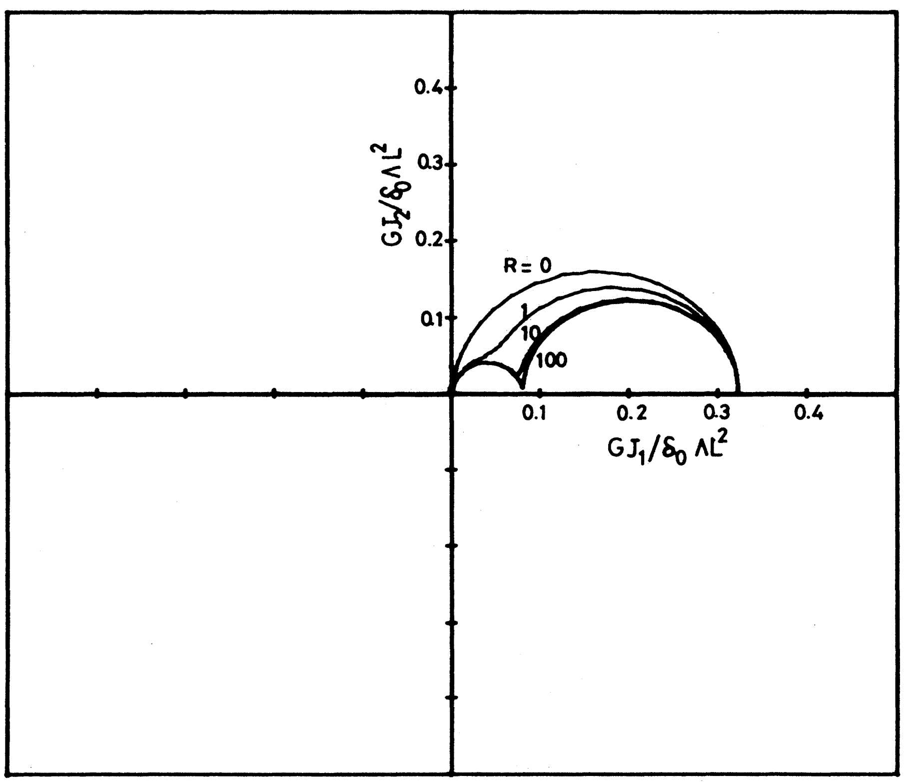

FIG. 3. The Cole-Cole diagrams for various values of the damping strength ratio are obtained from Eq. (17) and Eq. (18) using the parametric plotting technique. The decomposition of the original peak into the decoration peak and the parent peak (loop length $L/2$) is clearly seen in these diagrams.

the absence of the uniformly distributed dragging interstitials. The decoration peak maximum occurs at $\Omega_d = 4/\pi^2$ and the relaxation strength is about 76% of the standard Snoek-Koster relaxation peak. We should mention here that the standard Snoek-Koster peak is always assumed to be due to uniformly distributed interstitial atmospheres.

In Fig. 3 the Cole-Cole diagrams, which are obtained by plotting J_2 as a function of J_1 for the various values of the damping strength ratio R according to Eqs. (17) and (18), are presented. This figure clearly shows that the original relaxation spectrum associated with the uniformly distributed interstitials splits into two subpeaks upon decoration with heavy dragging-point defects. The relaxation strength of one peak is $\frac{1}{4}$ of the original peak, and the other subpeak has a relaxation strength of $\frac{3}{4}$.

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