Homogenization and Path Independence of the *J*-Integral in Heterogeneous Materials

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The J-integral that determines the driving force on a crack tip is a central concept of fracture mechanics. It is particularly useful since it is path independent in homogeneous materials. However, most materials are heterogeneous at a microscopic scale, and the J-integral is not necessarily path independent in heterogeneous media. In this paper, we prove the existence of an effective J-integral in heterogeneous media, show that it can be computed from the knowledge of the macroscopic or homogenized displacement fields and that it is path independent in macroscopically homogeneous media as long as the contours are large compared to the length scale of the heterogeneities. This result justifies the common engineering use of the J-integral. [DOI: 10.1115/1.4034294]

1 Introduction

It has been understood from the work of Griffith [1], Irwin [2], and others that the propagation of cracks is driven by the energy release rate, i.e., the rate of change of elastic energy with respect to crack extension. Rice [3] showed that this energy release rate may be described by the J-integral

$$J = \int_\Gamma t_i \left(W\delta_{ij} - \frac{\partial u_k}{\partial x_i}\sigma_{kj} \right) n_j ds \qquad (1)$$

where W is the stored energy density, u is the displacement, $\sigma = \partial W/\partial F$ the stress, n is the normal to the contour Γ enclosing the crack tip, and t is the tangent to the crack at the crack tip. Conveniently, the J-integral is path independent, i.e., it does not depend on the contour Γ as long as the medium is homogeneous. This makes it extremely useful, since one can choose contours along which it is most convenient to evaluate the integrand.

However, the J-integral is *not* necessarily path independent in heterogeneous materials. And most materials are heterogeneous at a microscopic scale. Still, the J-integral has proven to be a most useful concept. Typically, one notes that the scale of heterogeneities is small compared to the engineering object of interest, uses homogenization theory to define an effective elastic medium which is homogeneous at the engineering scale, and applies elasticity theory and the J-integral to this effective homogenous medium.

Unfortunately, the relation between a "microscopic" and "macroscopic" J-integral remains open. Specifically, it is not clear whether the J-integral computed with the stress and the strain associated with the heterogeneous medium will converge to the J-integral computed with the stress and the strain associated with the effective homogeneous medium as the contour becomes very large. In short, it is not clear whether one can use the solutions to the homogenized equation to compute an effective J-integral.

Indeed, a casual examination of the expression for the J-integral in Eq. (1) suggests that the microscopic J-integral will in general be different from the macroscopic or homogenized J-integral. While we know from homogenization theory (specifically Hill's Lemma [4]) that the average of the microscopic stored energy density is equal to the macroscopic stored energy density, this does not appear to be true for the second term in the parenthesis in the integrand of Eq. (1). Specifically, the stress and the displacement gradient fluctuate at the microscopic scale in a heterogeneous medium. Therefore, it is generally not true that the product of their averages is equal to the average of their products; in other words, it is unclear if

$$\left\langle \frac{\partial u_k}{\partial x_i} \right\rangle \langle \sigma_{kj} \rangle = \left\langle \frac{\partial u_k}{\partial x_i}\sigma_{kj} \right\rangle ? \qquad (2)$$

This raises an issue of using the J-integral in engineering practice.

Further, the recent decades have seen an attempt to use heterogeneities to enhance fracture toughness. Furthermore, nature exploits microstructure to enhance toughness of nacre and other shells. Finally, the emergence of 3D printing and other methods of additive material synthesis opens the possibility of exploiting carefully controlled heterogeneity for enhancing the toughness of materials. All of this has led to a new interest in understanding the effective toughness of heterogeneous media (see for example, Ref. [5] and references therein).

In this paper, we use homogenization theory in a quasi-periodic setting to show the existence of a macroscopic J-integral, and prove that this is path independent in a macroscopically homogeneous material if the path is large compared to the size of the heterogeneities. The path independence of the J-integral follows from the fact that it is closely related to the configurational stress tensor or the Eshelby energy momentum tensor

$$C_{ij} = W\delta_{ij} - \frac{\partial u_k}{\partial x_i}\sigma_{kj} \qquad (3)$$

that satisfies

$$\frac{\partial C_{ij}}{\partial x_j} = \frac{\partial^* W}{\partial^* x_i} \qquad (4)$$

where $\partial^*/\partial^* x_i$ denotes the explicit derivative with respect to x_i. This equation may be obtained from the equilibrium equation, and is also referred to as the *configurational force balance*. Integrating this equation over an annular region between two contours and using the divergence theorem leads to the path independence of the J-integral in homogeneous materials. We show that the homogenization of this equation retains the same form leading to a homogenized configurational stress tensor and homogenized J-integral.

We recall homogenization of the variational formulation of elasticity in Sec. 2 and derive our main result in Sec. 3. We conclude in Sec. 4.

2 Periodic Homogenization

Consider a domain Ω (a bounded open set in $\mathbb{R}^N$) with a heterogeneous elastic medium where the heterogeneities have a length

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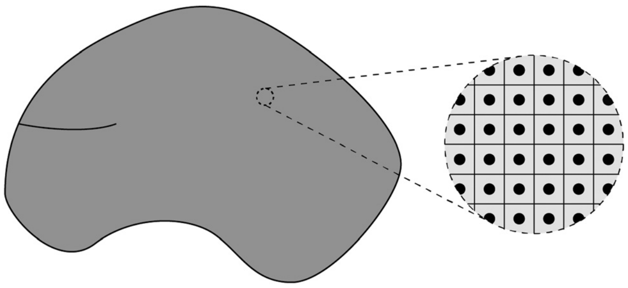

Fig. 1 A macroscopic crack in a quasi-periodic heterogeneous medium

scale $\varepsilon \ll 1 = \mathrm{diam}(\Omega)$ in dimensionless units. The domain may contain a smooth crack of whose length is $O(1)$. Specifically, we assume that the medium is *quasi-periodic* so that the stored energy density

$$\widetilde{W}^{\varepsilon}(F,x) = W\left(F, x, \frac{x}{\varepsilon}\right) \tag{5}$$

where F is the displacement gradient, $W : \mathbb{R}^{N\times N} \times \Omega \times Y \to \mathbb{R}$, Y is the unit cube in $\mathbb{R}^N$ and $W(F,x,y)$ is periodic in y for each x, F. This is shown schematically in Fig. 1: the medium appears periodic if we look closely at some point $x \in \Omega$.

In the case of linear elasticity

$$W(F,x,y) = \frac{1}{2}F_{ij}\mathbb{C}_{ijkl}(x,y)F_{kl} \tag{6}$$

where $\mathbb{C} : \Omega \times Y \to \mathbb{R}^{N^4}$ is the elastic modulus satisfying major and minor symmetries, and $\mathbb{C}(x,y)$ is periodic in y for each x.

We seek solutions of the equations of elasticity by seeking to minimize the total energy

$$\mathcal{E}^{\varepsilon}[u] = \int_{\Omega} \widetilde{W}^{\varepsilon}(\nabla u, x)dx - \mathcal{L}[u] = \int_{\Omega} W\left(\nabla u, x, \frac{x}{\varepsilon}\right)dx - \mathcal{L}[u] \tag{7}$$

where $\mathcal{L}$ depends on the body force and boundary tractions among all displacements $u : \Omega \to \mathbb{R}^3$ that satisfy the imposed displacement boundary conditions. This problem is difficult because W and consequently the solution oscillates on the scale of the heterogeneities ε. Homogenization theory [6,7] states that if ε is small enough and if $W(F,x,y)$ is convex in F for each x, y,[1] then we can replace the problem above with the following *effective problem*: minimize

$$\mathcal{E}[u] = \int_{\Omega} \overline{W}(\nabla u, x)dx - \mathcal{L}[u] \tag{8}$$

among all displacements that satisfy the imposed displacement boundary conditions where $\overline{W} : \mathbb{R}^{N\times N} \times \Omega \to \mathbb{R}$ is the effective elastic energy density and may be obtained by solving the following problem for each F, x: minimize

$$\overline{W}(F,x) = \int_Y W(F + \nabla\varphi(y), x, y)dy \tag{9}$$

overall periodic displacement fields $\varphi : Y \to \mathbb{R}^N$. Note that the integrand of Eq. (8) is smooth on the scale of ε and thus the solution is also expected to be smooth at that scale. It is also true that the effective stress is given by

$$\overline{\sigma}_{ij} = \frac{\partial \overline{W}}{\partial F_{ij}} \tag{10}$$

Further, under suitable growth and strict convexity conditions on W, the minimum is attained and unique up to an inessential translation. We call the minimum $\varphi^{F,x}$. So

$$\mathcal{E}[u] = \int_{\Omega}\int_{Y} W(\nabla_x u + \nabla_y \varphi^{\nabla_x u, x}, x, y)dydx - \mathcal{L}[u] \tag{11}$$

3 Configurational Force Balance

We use the effective functional (11) to derive an effective configurational force balance. We take $\mathcal{L} = 0$ for convenience (i.e., no body force, and traction-free and displacement boundary conditions), but the treatment is easily modified otherwise.

Let $\overline{u}$ minimize $\mathcal{E}$ defined in Eq. (11) for some given boundary conditions. Recall that it is smooth on the scale of ε. We now consider a variation, but by rearranging the domain.[2] Consider a family of rearrangments $z^s : \Omega \to \Omega$ one to one and onto for $s \in [0,1]$ that satisfy $z = x$ on $\partial\Omega$, $\det\nabla_x z > 0\, \forall x \in \Omega$, and $z^0(x) = x$. Set $\overline{u}^s(x) = \overline{u}(z^s(x))$. Note that $\overline{u}^s$ is a family of perturbations of the minimizer $\overline{u}$ with $\overline{u}^0 = \overline{u}$. Therefore, the function

$$f(s) := \mathcal{E}[\overline{u}(z^s)] \tag{12}$$

has a minimum at $s = 0$ and therefore

$$f'(0) = 0 \tag{13}$$

We now compute $f'(0)$.

Set $\psi^s = \varphi^{\nabla_x \overline{u}^s, x}$ and $\overline{F}(x) = \nabla_x \overline{u}(x)$, and note that

$$\nabla_x \overline{u}^s = \nabla_x(\overline{u}(z^s(x))) = \overline{F}(z^s(x))\nabla_x z^s(x) \tag{14}$$

So

$$f(s) = \int_{\Omega}\int_{Y} W(\overline{F}(z^s(x))\nabla_x z^s + \nabla_y \psi^s, x, y)dydx \tag{15}$$

$$= \int_{\Omega}\int_{Y} W(\overline{F}(z)(\nabla_z x^s)^{-1} + \nabla_y \psi^s, x^s, y)Jdydz \tag{16}$$

where we have changed integration variables from x to z by inverting z^s to obtain $x = x^s(z)$, and set $J = \det(\nabla_z x^s)$. Now, set

$$\overline{F}^s = \overline{F}(z)(\nabla_z x^s)^{-1}, \quad G^s = \overline{F}^s + \nabla_y \psi^s = \overline{F}^s + \nabla_y \varphi^{\overline{F}^s, x^s} \tag{17}$$

We can now calculate

$$f'(s) = \int_{\Omega}\int_{Y} \left(\frac{\partial W}{\partial F_{ij}}\dot{G}^s_{ij} + \frac{\partial^* W}{\partial^* x_i}\dot{x}_i + W\frac{\dot{J}}{J}\right)Jdydz \tag{18}$$

where we use $\partial^*/\partial^* x_i$ to represent the explicit derivative with respect to x_i and $\dot{(q)} = dq/ds$ to denote the total derivative of q with respect to s. Recalling the identities

$$\dot{\overline{A^{-1}}} = -A^{-1}\dot{A}A^{-1}, \quad \dot{\overline{\det A}} = (\det A)A^{-T}_{ij}\dot{A}_{ij} \tag{19}$$

we obtain

$$\dot{G}^s_{ij} = \dot{\overline{F}}^s_{ij} + \frac{\partial \dot{\psi}^s_i}{\partial y_j} = -\overline{F}_{ik}(z)\left(\frac{\partial x^s_k}{\partial z_l}\right)^{-1}\frac{\partial \dot{x}^s_l}{\partial z_m}\left(\frac{\partial x^s_m}{\partial z_j}\right)^{-1} + \frac{\partial \dot{\psi}^s_i}{\partial y_j} \tag{20}$$

[1]This holds true for common linear elastic problems. Failure of this condition may lead to long-range instabilities.

[2]Such variations are known as *inner variation* in the calculus of variations.

$$\frac{\dot{J}}{J} = \left(\frac{\partial x_i^s}{\partial z_j}\right)^{-T}\left(\frac{\partial \dot{x}_i^s}{\partial z_j}\right)^{-1} \tag{21}$$

Further, from the unit cell problem of minimizing (9), we can infer that

$$\int_Y \frac{\partial W}{\partial F_{ij}}\frac{\partial \dot{\psi}_i^s}{\partial y_j}dy = 0 \tag{22}$$

We substitute Eqs. (20)–(22) into Eq. (18), set $s=0$ (so that $\partial x_i^s/\partial z_j = \delta_{ij}$) and change integration variables back to x

$$f'(0) = \int_\Omega\int_Y \left(\left(W\delta_{ik} - \frac{\partial W}{\partial F_{ij}}\overline{F}_{ik}\right)\frac{\partial \dot{x}_k}{\partial x_j} + \frac{\partial^* W}{\partial^* x_k}\dot{x}_k\right)dydx \tag{23}$$

where $\dot{x} = \dot{x}^s(z)|_{s=0}$. We note that $\overline{F}$ and $\dot{x}$ are independent of y and therefore we can integrate with respect to y. We obtain by recalling (9)

$$f'(0) = \int_\Omega \left(\left(\overline{W}\delta_{ik} - \frac{\partial \overline{W}}{\partial F_{ij}}\overline{F}_{ik}\right)\frac{\partial \dot{x}_k}{\partial x_j} + \frac{\partial^* \overline{W}}{\partial^* x_k}\dot{x}_k\right)dx \tag{24}$$

$$= \int_\Omega \left(-\frac{\partial}{\partial x_j}\left(\overline{W}\delta_{ik} - \frac{\partial \overline{W}}{\partial F_{ij}}\overline{F}_{ik}\right) + \frac{\partial^* \overline{W}}{\partial^* x_k}\dot{x}_k\right)\dot{x}_k dx \tag{25}$$

where we have used the divergence theorem and the fact that $\dot{x} = 0$ on $\partial\Omega$ (since $x = z^s(x)$ on $\partial\Omega$). Now, since $f'(0) = 0$ for all z^s and thus arbitrary $\dot{x}$, we obtain the macroscopic *configurational force balance*

$$\frac{\partial \overline{C}_{ij}}{\partial x_j} = \frac{\partial^* \overline{W}}{\partial^* x_i} \tag{26}$$

where

$$\overline{C}_{ij} = \overline{W}\delta_{ij} - \overline{F}_{ki}\frac{\partial \overline{W}}{\partial F_{kj}} = \overline{W}\delta_{ij} - \overline{F}_{ki}\overline{\sigma}_{kj} \tag{27}$$

is the effective configurational stress tensor.

Finally, if the material is macroscopically homogeneous, i.e., W and consequently $\overline{W}$ is independent of x, then we see from Eq. (26) that

$$0 = \int_D \frac{\partial \overline{C}_{ij}}{\partial x_j}dx = \int_{\partial D} \overline{C}_{ij}n_j dA \tag{28}$$

using the divergence theorem where D is any domain that is large compared to the size of the heterogeneities (ε). Now, consider a domain with a crack in two dimensions. Given any two contours Γ_1 and Γ_2 that contain the crack tip, set D to be the annular region between the contours. Now, $\partial D = \Gamma_1 \cup \Gamma_2$ with the outward normal $-n$ and n on the two segments of the boundary. Taking the inner product of the equation above with the tangent to the crack tip, we obtain

$$\int_{\Gamma_1} t_i\left(\overline{W}\delta_{ij} - \frac{\partial \overline{u}_k}{\partial x_i}\overline{\sigma}_{kj}\right)n_j ds = \int_{\Gamma_2} t_i\left(\overline{W}\delta_{ij} - \frac{\partial \overline{u}_k}{\partial x_i}\overline{\sigma}_{kj}\right)n_j ds \tag{29}$$

or the path independence of the macroscopic J-integral.

4 Conclusion

We have shown the existence of a homogenized configuration stress tensor and configurational force balance in a quasi-periodic medium. We have used these to show the existence of an effective J-integral that may be evaluated from the macroscopic displacements and stresses, and that is path independent in macroscopically homogeneous media as long as the contours are large enough.

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