Two State M-Integral Analysis for a Nano-Inclusion in Plane Elastic Materials Under Uni-Axial or Bi-Axial Loadings

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In this paper, the two state M-integral is extended from macrofacture to nanodefect mechanics. The question as to why the M-integral for a nanovoid or a soft nano-inclusion might be negative is clarified. It is concluded that the surface tension plays a dominant role in evaluating the M-integral, whereas the surface Lamè constants yield much less influence than the surface tension. Their influence on the M-integral for a nanovoid or a soft nano-inclusion could be neglected. [DOI: 10.1115/1.3176998]

Keywords: The two state M-integral, Mode decomposition, Nano-inclusion, Surface tension, Surface Lamè constants

1 Introduction

The concept of the two state conservation integral such as the two state J-integral or the two state M-integral was introduced in classical fracture mechanics to distinguish the mixed mode stress intensity factors (SIFs) at a macrocrack tip. Chen and Shield [1] might be the first who established three conservation laws for two 2equilibrium states and called them the two state conservation integrals. Subsequently, the two state integrals were widely employed to calculate SIFs and the elastic T-stresses ahead of a crack tip [2–10]. The key of this concept is the so-called mode decomposition. In nanodefect mechanics, to the authors' knowledge, the two state conservation integral has not been used in literature.

In this paper, the two state M-integral is extended to treat nanodefect problems. The overall M-integral for the original elastic field for a nanovoid is divided into three distinct terms, which are contributed by the elastic field induced from the external loading, the elastic field induced from the surface parameters along a nanovoid or soft nano-inclusion, and the intersecting term induced from the interaction between the two former elastic fields.

It is concluded that whether the M-integral for a nanovoid is negative depends on the intersecting term. Mathematically, the negative values of the M-integral mean that the interacting effect between the two elastic fields is larger than the effect induced from the external loading only. Detailed numerical results reveal that the surface tension plays a dominant role in evaluating the M-integral under the two different kinds of loading. Thus, the simple and approximate relations between the M-integral and the surface tension are presented for the nanovoid, which merely lead to some small errors in a tolerant way.

2 The Two State M-Integral

In this section, the two state M-integral is adopted in nanoscale. A decomposition of the original elastic field with a nano-inclusion obtained in Ref. [1] is performed and then

$$\sigma_{xx} = \sigma_{xx}^{(1)} + \sigma_{xx}^{(2)}, \quad \sigma_{yy} = \sigma_{yy}^{(1)} + \sigma_{yy}^{(2)}, \quad \sigma_{xy} = \sigma_{xy}^{(1)} + \sigma_{xy}^{(2)} \tag{1}$$

$$u_x = u_x^{(1)} + u_x^{(2)}, \quad u_y = u_y^{(1)} + u_y^{(2)} \tag{2}$$

where the superscript (1) represents the quantities under the purely external loading without any consideration of the surface parameters along the nano-inclusion (see Fig. 1) and the superscript (2) represents the quantities under the surface parameters along the nanovoid only without any external loading.

According to the work of Chen and Shield [1], the overall M-integral should be the summation of the following three terms:

$$M = M^{(1)} + M^{(2)} + M^{(1,2)} \tag{3}$$

where the first two terms $M^{(1)}$ and $M^{(2)}$ correspond to fields "(1)" and "(2)," respectively, as formulated below

$$M^{(1)} = \oint_C (w^{(1)} x_i e_i - T_k^{(1)} u_{k,i}^{(1)} x_i) ds \tag{4}$$

$$M^{(2)} = \oint_C (w^{(2)} x_i e_i - T_k^{(2)} u_{k,i}^{(2)} x_i) ds \tag{5}$$

which can be calculated by using the solutions presented in Ref. [11] without any difficulty.

Setting the three surface parameters to be zero in the basic formulations of Ref. [11] yields the explicit expression of $M^{(1)}$, which should be the same as those for a macrocircular inclusion in an infinite elastic plane

$$M^{(1)} = \frac{\pi(\kappa+1)R^2p^2}{4\mu}\left\{\frac{(\mu-\mu_1)}{(\mu+\kappa\mu_1)} + \frac{\mu(\kappa_1-1)+(1-\kappa)\mu_1}{2[\mu(\kappa_1-1)+2\mu_1]}\right\} \quad \text{(under the uni-axial tension loading)} \tag{6}$$

$$M^{(1)} = -\frac{\pi R^2(1+\kappa)[-19(\kappa_1-1)\mu^2 + (-55-\kappa(\kappa_1-2)+18\kappa_1)\mu\mu_1 + (36-\kappa+\kappa^2)\mu_1^2]p^2}{32\mu[(\kappa_1-1)\mu+2\mu_1](\mu+\kappa\mu_1)} \quad \text{(under the bi-axial tension compression loading)} \tag{7}$$

where μ and κ are the elastic constants of the matrix, μ_1 and κ_1 are the elastic constants of the inclusion, and R and p are the radius of the inclusion and the magnitude of the loading, respectively.

Alternatively, setting the external loading to be zero in the basic formulations of Ref. [11] yields the value of $M^{(2)}$. After doing so, it is obvious that the second term $M^{(2)}$ on the right hand side of Eq. (3) does vanish without any doubt

$$M^{(2)} \equiv 0 \tag{8}$$

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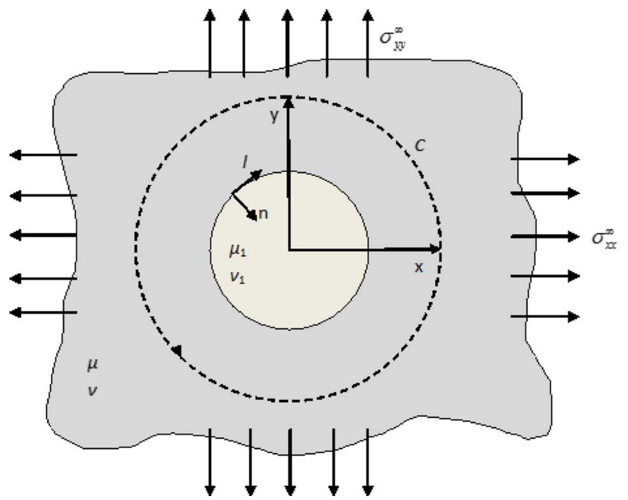

Fig. 1 Configuration of a nano-inclusion under the bi-axial loading

Thus, attention should only be focused on the third term on the right hand side of Eq. (3), which represents the interaction between the physical quantities in field (1) and those in field (2). The detailed expression of $M^{(1,2)}$ can be given as follows:

$$M^{(1,2)} = \oint_C \left\{ w^{(1,2)} x_i e_i - \left[T_x^{(1)} \left(\frac{\partial u_x^{(2)}}{\partial y} y + \frac{\partial u_x^{(2)}}{\partial x} x \right) + T_x^{(2)} \left(\frac{\partial u_x^{(1)}}{\partial y} y + \frac{\partial u_x^{(1)}}{\partial x} x \right) + T_y^{(1)} \left(\frac{\partial u_y^{(2)}}{\partial x} x + \frac{\partial u_y^{(2)}}{\partial y} y \right) + T_y^{(2)} \left(\frac{\partial u_y^{(1)}}{\partial x} x + \frac{\partial u_y^{(1)}}{\partial y} y \right) \right] \right\} ds \tag{9}$$

where the superscripts (1) and (2) represent the corresponding quantities defined in the stress displacement fields (1) and (2), respectively.

Substituting Eqs. (1) and (2) into Eq. (9) directly yields the following explicit formulation of the strain energy density in Eq. (9):

$$w^{(1,2)} = \tfrac{1}{2}[(\sigma_{xx}^{(1)}\varepsilon_{xx}^{(2)} + \sigma_{xx}^{(2)}\varepsilon_{xx}^{(1)}) + (\sigma_{yy}^{(1)}\varepsilon_{yy}^{(2)} + \sigma_{yy}^{(2)}\varepsilon_{yy}^{(1)}) + 2(\sigma_{xy}^{(1)}\varepsilon_{xy}^{(2)} + \sigma_{xy}^{(2)}\varepsilon_{xy}^{(1)})] \tag{10}$$

which can be calculated without any difficulty.

Obviously, when the μ_1 and κ_1 vanish, i.e., corresponding to a void, the first term $M^{(1)}$ on the right hand side of Eq. (3) should always be positive due to the energy release for the void expansion under the purely external loading without the surface effect, whereas the third term formulated by Eq. (9), called the intersecting term, is unclear at present. Thus, whether the overall the M-integral is negative depends on the difference between the first term $M^{(1)}$ and the third term $M^{(1,2)}$. Bear in mind that the positive value of the M-integral corresponds to the energy release due to the void expansion as those in the classical macrofracture mechanics, whereas the negative value of the M-integral corresponds to the energy absorbing due to the void expansion, which shows a quite different feature from the classical macrodefect mechanics. Detailed numerical results for the two state M-integral, especially $M^{(1,2)}$, should be presented to facilitate the better understanding for why or how the M-integral is negative in nanodefect mechanics.

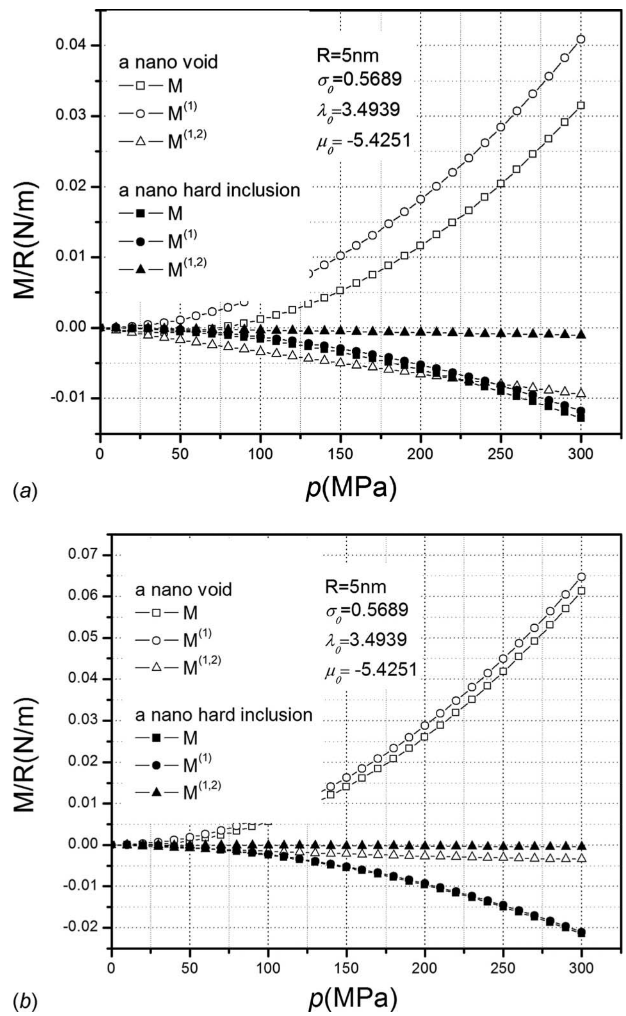

Fig. 2 Two terms $M^{(1)}$ and $M^{(1,2)}$ for a nanovoid and a nanohard inclusion with R=5 nm: (*a*) uni-axial tension loading and (*b*) bi-axial tension compression loading

3 Numerical Results

First, the numerical results of the two terms $M^{(1)}$ and $M^{(1,2)}$ for a nanovoid and a hard nano-inclusion with $R=5$ nm and $\mu_0=-5.4251$ N/m, $\lambda_0=3.4939$ N/m, and $\sigma_0=0.5689$ N/m [12], under the two kinds of loading, are plotted in Figs. 2(*a*) and 2(*b*), respectively. Here, Fig. 2(*a*) refers to the uni-axial tension loading with $\sigma_{yy}^{\infty}=p$ and $\sigma_{xx}^{\infty}=0$, whereas Fig. 2(*b*) refers to the bi-axial tension compression loading with $\sigma_{yy}^{\infty}=p$ and $\sigma_{xx}^{\infty}=-p/2$ (see Fig. 1). It is seen from Fig. 2(*a*) that the values of $M^{(1,2)}$ with the symbol △ are always negative, whereas the values of $M^{(1)}$ with symbol ○ are always positive. Thus, the overall M-integral for a nanovoid can be either positive or negative depending on the difference between $M^{(1)}$ and $M^{(1,2)}$. $M^{(1)}>|M^{(1,2)}|$ yields the positive value of the overall M-integral and $M^{(1)}<|M^{(1,2)}|$ yields the negative value. Here, $M^{(1)}=|M^{(1,2)}|$ refers to the *neutral loading point* (about 70 MPa). When the uni-axial loading for the nanovoid is less than the neutral loading point, the positive $M^{(1)}$ is less than the magnitude of the negative $M^{(1,2)}$ and then the overall M-integral is negative, representing the energy absorbing due to the void expansion, whereas when the uni-axial loading increases over the neutral loading point, the positive $M^{(1)}$ becomes larger and larger than the magnitude of the negative $M^{(1,2)}$ and then the overall M-integral becomes positive, representing the energy release due to the void expansion. As regards the hard inclusion, it is seen from Fig. 2(a) that both $M^{(1)}$ with symbol ● and $M^{(1,2)}$ with symbol ▲ are negative and the magnitude of $M^{(1)}$ is always much larger than that of $M^{(1,2)}$. In other words, as compared with $M^{(1)}$, the interaction between the uni-axial loading and the surface parameters for a hard inclusion yields very small contribution to the $M^{(1,2)}$, which could be neglected. Figure 2(b) shows the variable tendencies of the overall M-integrals $M^{(1)}$ and $M^{(1,2)}$ under the bi-axial tension compression loading. It is seen that the interaction between the bi-axial tension compression loading and the surface parameters for the nanovoid yields very small contribution to $M^{(1,2)}$ with symbol △, which could be neglected as compared with $M^{(1)}$ with symbol ○. Thus, in most contents, the overall M-integral with symbol □ for the nanovoid is positive in Fig. 2(b), except those when the loading level is very low, e.g., $p < 37$ MPa. It is concluded that the horizontal compression loading yields significant effect to decrease the intersecting term $M^{(1,2)}$. For example, when the horizontal compression loading is half of the external vertical tension loading, as shown in Fig. 2(b), the intersecting term $M^{(1,2)}$ for the nanovoid becomes very small as compared with $M^{(1)}$, which could also be neglected. As regards to the hard nano-inclusion under the bi-axial tension compression loading, Fig. 2(b) shows similar results as those in Figs. 2(a). That is, both $M^{(1)}$ and $M^{(1,2)}$ are negative and $|M^{(1)}| \gg |M^{(1,2)}|$ so that the intersecting term $M^{(1,2)}$ could be neglected.

Second, the two terms of the M-integrals, $M^{(1)}$ and $M^{(1,2)}$ for a soft nano-inclusion and a rigid nano-inclusion with $R=5$ nm and $\mu_0=-5.4251$ N/m, $\lambda_0=3.4939$ N/m, and $\sigma_0=0.5689$ N/m under the two kinds of loading are plotted in Figs. 3(a) and 3(b), respectively. It is seen from Figs. 3(a) and 3(b) that the values of $M^{(1,2)}$ with symbol △ are always negative too as those in Figs. 2(a) and 2(b). It is concluded that whether the overall M-integral is negative for a soft nano-inclusion depends on the negative value of the intersecting term $M^{(1,2)}$ induced from the interaction between the two stress displacement fields of the external loading and the surface parameters in nanoscale. In other words, $M^{(1)} < |M^{(1,2)}|$ yields the negative value of the overall M-integral. In addition, for the rigid inclusion, Figs. 3(a) and 3(b) show that the intersecting term $M^{(1,2)}$ with symbol ▲ always vanish and then have no contribution to the overall M-integral.

It is useful to clarify which surface parameter among the three ones μ_0, λ_0, and σ_0 is the dominant parameter governing the variable tendencies of the M-integral for a nanovoid. Numerical results for the 5 nm void are shown in Figs. 4(a) and 4(b) under the two kinds of loading. The surface parameters $\mu_0=-5.4251$ N/m, $\lambda_0=3.4939$ N/m, and $\sigma_0=0.5689$ N/m are used [11,12] and three additional cases $\mu_0=0$, $\lambda_0=3.4939$ N/m, and $\sigma_0=0.5689$ N/m, $\mu_0=-5.4251$ N/m, $\lambda_0=0$, and $\sigma_0=0.5689$ N/m, and $\mu_0=0$, $\lambda_0=0$, and $\sigma_0=0.5689$ N/m are considered for making comparisons. It is clearly shown in Figs. 4(a) and 4(b) that the four curves with the same value of $\sigma_0=0.5689$ N/m and with so different values of μ_0 and λ_0 almost coincide very well. It is concluded that the surface tension σ_0 is the dominant parameter governing the variable tendencies of the M-integral for the nanovoid under each of the two kinds of loading, whereas the other two parameters, i.e., surface Lamè constants μ_0 and λ_0, yield quite small influence on the values of the M-integral as compared with those induced from the surface tension σ_0 only, i.e., $\mu_0=0$, $\lambda_0=0$, and $\sigma_0=0.5689$ N/m. Numerical results shown in Figs. 4(a) and 4(b) reveal that the relative errors between the two curves with symbol ▽ and those with symbol ■ are always very small, i.e., less than 3%.

It should be mentioned that the numerical results in finding the dominant parameter in evaluating the M-integral arising from the another set of surface parameters [11,12], $\mu_0=-0.3760$ N/m, $\lambda_0=6.8511$ N/m, and $\sigma_0=0.9108$ N/m, are also calculated by considering the three additional cases $\mu_0=0$, $\lambda_0=6.8511$ N/m, and $\sigma_0=0.9108$ N/m; $\mu_0=-0.3760$ N/m, $\lambda_0=0$, and $\sigma_0=0.9108$ N/m; and $\mu_0=0$, $\lambda_0=0$, and $\sigma_0=0.9108$ N/m, respectively. The conclusions obtained from the second set of surface parameters are almost the same as those obtained above from the first set of surface parameters.

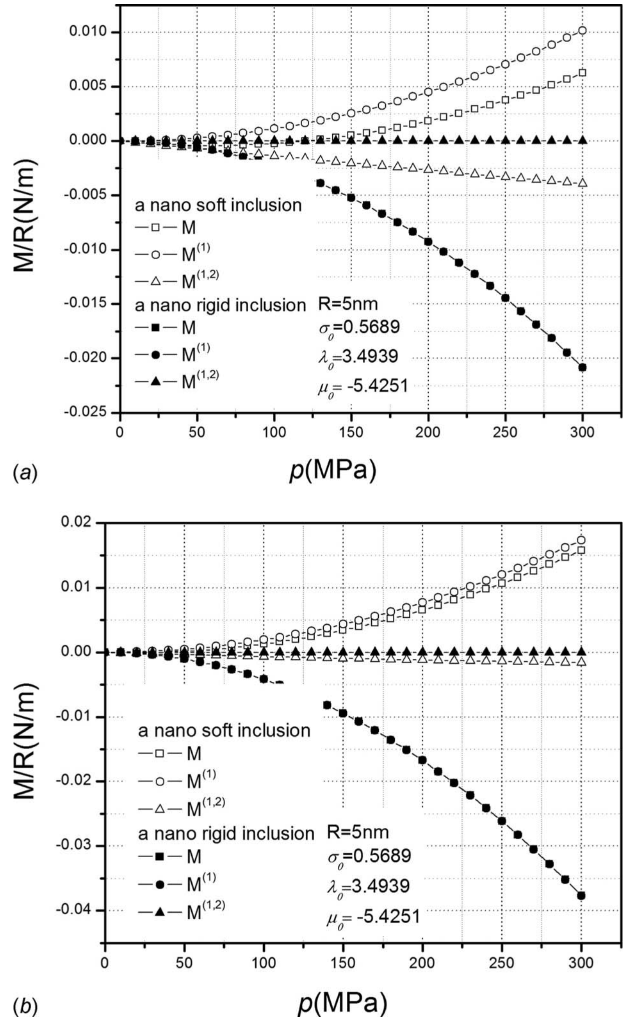

Fig. 3 Two terms $M^{(1)}$ and $M^{(1,2)}$ for a nanosoft inclusion and a nanorigid inclusion with $R=5$ nm: (a) uni-axial tension loading and (b) bi-axial tension compression loading

Since the surface tension for the nanovoid plays the dominant role in calculating the M-integral and the contribution induced from the surface Lamè constants μ_0 and λ_0 could be neglected in general. There should be some simple or approximate relations between the M-integral and the surface tension for the nanovoid under the two kinds of loading. After some simple manipulations, these approximate relations are cited below

$$M = \frac{p\pi R(3pR - 2\sigma_0)(1-\nu)}{2\mu} \quad \text{(under uni-axial-tension with } \sigma_{yy}^{\infty}=p) \tag{11}$$

$$M = \frac{p\pi R(19pR - 4\sigma_0)(1-\nu)}{8\mu} \quad \text{(under bi-axial-tension compression with } \sigma_{yy}^{\infty}=p \text{ and } \sigma_{xx}^{\infty}=-p/2) \tag{12}$$

Mathematically, these formulations significantly simplify the calculation of the M-integral for the nanovoid. Bear in mind that such simplification will yield some relative errors induced from neglecting the two surface Lamè constants μ_0 and λ_0 but these errors in general are in a tolerant way. Moreover, it is interest to

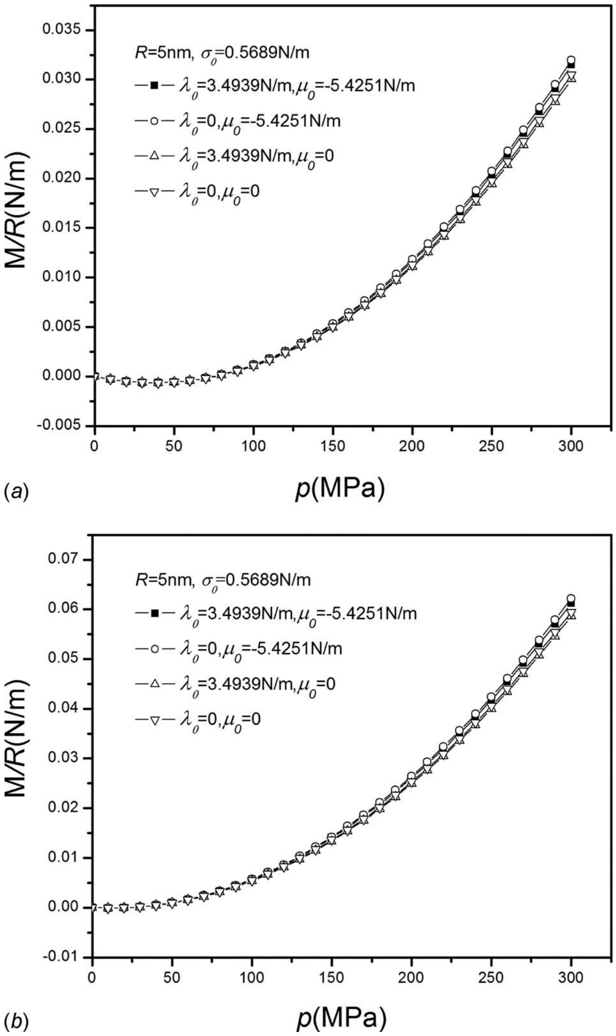

Fig. 4 The influence of different surface Lamè constants (λ_0, μ_0) on the *M*-integral for a nanovoid with $R=5$ nm: (*a*) uni-axial tension loading and (*b*) bi-axial tension compression loading

find from Eqs. (11) and (12) that whether the M-integral is negative mainly depends on the difference $3pR-2\sigma_0$ in Eq. (11) and the difference $19pR-4\sigma_0$ in Eq. (12). From the mathematical point of view, this finding provides a simple way to explain why the values of the M-integral could be either positive or negative for a void under the two kinds of loading as found in Ref. [11]. Indeed, when the loading level p is small, the differences $3pR-2\sigma_0$ and $19pR-4\sigma_0$ will be negative so that the M-integral should be negative, representing the energy absorbing due to void expansion. Alternatively, when the loading level p is large, the differences $3pR-2\sigma_0$ and $19pR-4\sigma_0$ will be positive so that the M-integral should be positive, representing the energy release due to void expansion.

Of great interest is that the neutral loading point at which the M-integral varies from a positive value to a negative value could be determined approximately by using the simplified formulations (Eqs. (11) and (12)). For example, under the bi-axial tension compression loading, the neutral loading point could be determined by setting $19pR-4\sigma_0=0$ in Eq. (12) approximately corresponding to 24 MPa for $\sigma_0=0.5689$ N/m and $R=5$ nm or approximately corresponding to 37 MPa for $\sigma_0=0.9108$ N/m and $R=5$ nm. These two values 24 MPa and 37 MPa coincide well or approximately with those obtained from the detailed formulations in Ref. [11], i.e., 24 MPa and 38 MPa.

4 Conclusions and Remarks

The concept of the two state M-integral classically adopted in macrofracture mechanics is very useful in treating the nano-inclusion problems. The M-integral for the whole elastic field with a nano-inclusion which is divided into three distinct terms, namely, $M^{(1)}$, $M^{(2)}$, and $M^{(1,2)}$, contributed to the external loading, the surface parameters, and the intersection between the two elastic fields mentioned above. It is concluded that the second term $M^{(2)}$ does always vanish, i.e., the surface parameters themselves have no contribution to the M-integral in nanodefect mechanics. Thus, whether the M-integral for a nanosoft inclusion or nanovoid is negative depends only on the difference between $M^{(1)}$ and $M^{(1,2)}$. Numerical results reveal that the values of $M^{(1,2)}$ for a nanosoft inclusion or void are always negative no matter how large the uni-axial tension loading or bi-axial loading is, whereas the values of $M^{(1)}$ are always positive. Thus, $M^{(1)}>-M^{(1,2)}$ yields the positive values of the M-integral, representing the energy released due to the soft inclusion or void expansion and $M^{(1)}<-M^{(1,2)}$ yields the negative values of the M-integral, representing the energy absorbed due to the soft inclusion or void expansion, whereas the neutral loading point occurs when $M^{(1)}=-M^{(1,2)}$, at which the M-integral transforms from a negative value to a positive value. Moreover, detailed numerical results reveal that the influences of the three surface parameters μ_0, λ_0, and σ_0 for the nanosoft inclusion and void on the M-integral are quite different and that the surface tension σ_0 plays a dominant role in evaluating the M-integral, whereas the other two parameters μ_0 and λ_0 yield much smaller influence on the M-integral, which could be neglected in general. The simple and approximate formulations between the M-integral and the surface tension for a nanovoid is presented by neglecting the influence of the surface Lamè constants, i.e., setting $\lambda_0=0$ and $\mu_0=0$. It is concluded that this approximation is tolerant with the relative errors less than 3% in the two kinds of loading mentioned above, provided that the loading level is not too high, e.g., less than 150 MPa. Even though the loading level is large as 300 MPa, the relative errors of the M-integral induced from neglecting surface Lamè constants are less than 5% under each of the two kinds of loading mentioned above. In addition, the surface parameters for a nanohard inclusion or rigid inclusion have a little or little influence on the M-integral and the values of the M-integral are always negative and both $M^{(1)}$ and $M^{(1,2)}$ are negative with $|M^{(1)}|\gg|M^{(1,2)}|$.

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