THE RDA MODEL OF SCALING AND SIZE EFFECT OF NANOCOMPOSITES

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Abstract: This paper presents an application of the rheological-dynamical analogy (RDA) for predicting new notch stress intensities of nano-structured composites. The analogy has been developed on the basis of mathematical-physical analogy between a visco-elasto-plastic rheological model and a dynamic model with viscous damping, and is aimed to be used for the analysis of inelastic deforming of materials. Bohr's quantum model of the atom and de Broglie wave hypothesis for matter is used for the RDA model of a diatomic molecule. The model is also confirmed by the classical Griffith's theory of fracture in an infinite plate loaded by a normal stress.

Key words: nanocomposites, RDA model, critical fracture stresses

RDA MODEL RAZMJERA I EFEKTA VELIČINE KOD NANOKOMPOZITA

Sažetak: Ovaj rad predstavlja primjenu reološko-dinamičke analogije (RDA) za predviđanje novih intenziteta naprezanja zareza nano-strukturiranih kompozita. Analogija je razvijena na temelju matematičko-fizičke analogije između viskoelastoplastičnog reološkog modela i dinamičkog modela s viskoznim prigušenjem, a namijenjena je da se koristi za analizu neelastičnog deformiranja materijala. Za RDA model dvoatomske molekule koristi se Bohrov kvantni model atoma i de Broglie-va valna hipoteza za materiju. Model je potvrđen i klasičnom Griffithovom teorijom loma u beskonačnoj ploči opterećenoj normalnim naprezanjem.

Ključne riječi: nanokompoziti, RDA model, kritična naprezanja loma

1. INTRODUCTION

Although experimental-based research can ideally be used to determine structure-property relationships of materials and nano-structured composites at the macro and at the atomic scale, experimental synthesis and characterization of composite strengths demands the use of sophisticated processing methods and testing equipment; which could result in exorbitant costs. Nanocrystalline (n) materials i.e. polycrystalline materials, are of considerable scientific and technological interests. Because of the complex interactions between constituent phases at the atomic level, a combination of modeling techniques is often required to simulate the bulk-level behavior of these materials, see Odegard et.al [4]. The computational chemistry techniques assume the presence of a discrete molecular structure, and are primarily used to predict the atomic structure of a material. Computational mechanics techniques assume that the matter is composed of one or more continuous constituents, and are used to predict the mechanical behavior of materials and structures. These two types of modeling techniques must be combined to an overall multiscale model that is capable of predicting the structure and properties of n-materials based on fundamental and scientific principles.

2. THE RDA ANALOGY AT THE MACRO SCALE

Each isochronous stress-strain diagram of a thin long symmetrical bar at the macro scale, Fig. 1 can be accurately approximated by the rheological equation

$$\text{H—K—(N|StV)} \tag{1}$$

The governing differential equation has already been derived and solved on harmonic excitation by Milašinović [2] using by based RDA equations:

$$m = \frac{a_K a_N}{¥} = kT_K^{D^2},\ c = \frac{\left(E_K a_N + H' a_K\right)}{¥} = 2kT_K^D,$$
$$k = \frac{E_K H'}{¥} \tag{2}$$

T_K^D represent a characteristic time (dynamical time of retardation): the time a wave velocity c takes to propagate length l_0 of the bar.

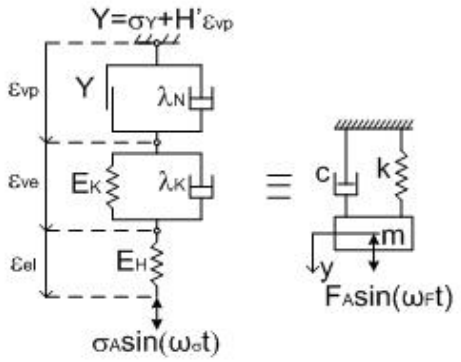

Figure 1. Rheological-dynamical analogy (RDA)

3. THE RDA SIZE EFFECT AT THE ATOMIC SCALE

Fracture fundamentally has to do with the severing of atomic bonds: this points theoretical investigations toward atomic scale studies.
Unless excited by external means, the one electron of Bohr's quantum model of a hydrogen atom will occupy the lowest orbit (r_1=0.0529nm). De Broglie argued that only those electron waves which formed circular standing waves and hence, could reinforce themselves would form orbits. The condition for forming a circular standing wave is that the wavelength (λ) fits into the circumference of the orbit an integer number of times. Consequently, for *n=1*

$$a = 2\pi r_1 \tag{3}$$

Using the description of the free longitudinal vibration of a diatomic molecule (Fig. 2), the natural frequencies may be determined as follows:

$$\sin\left(\frac{p_i a}{c}\right) = 0 \Rightarrow p_i = i\pi\frac{c}{a}, i = 1,2,3,...,\infty \tag{4}$$

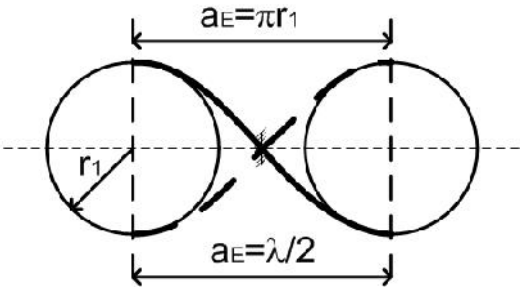

Figure 2. Standing mater wave of a diatomic molecule

The first case of resonance (standing wave) occurs when the characteristic distance for given pair of atoms is half the length of a matter wave

$$a_E = \frac{a}{2} = \pi r_1 \tag{5}$$

Substituting the characteristic distance πr_1 into the Eq. (4) we obtain the natural frequency of the atom having vibration in his position of lowest energy

$$p_1 = f = \pi\frac{c}{\pi r_1} = \frac{c}{r_1} = \frac{1}{r_1}\sqrt{\frac{E_H}{m}} \tag{6}$$

In the special case at creep coefficient $\varphi^* \to 0$ (state of elasticity without of the reduction of the cross-section area of the bar, $\Phi/\Phi_{red}=1$) we have the cyclic toughness obtained by Milašinović [2] as follows

$$G_I = \frac{\sigma_A^2 \pi r_1}{E_H} \tag{7}$$

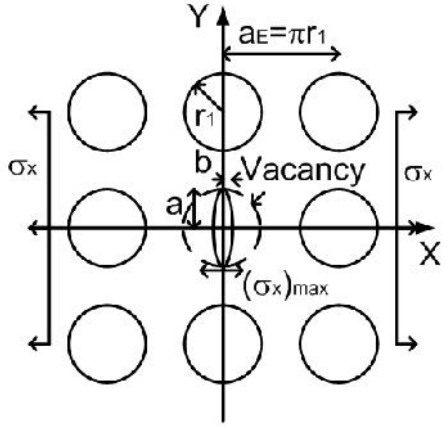

Figure 3. The classical Griffith's crack according to the RDA analogy of a diatomic molecule

Griffith [1] used the solution of Inglish to show that the rate of release of potential energy, G_I, with respect to the crack area, *2aB*, in an infinite plate loaded by a normal stress, σ, is given by Eq. (7). *B* is the thickness of the plate and minimal crack length *2a* is equal to the diameter of one vacancy $2r_1$, as shown in Fig. 3. If the specific surface energy is *y* the necessary condition gives the critical fracture stress at the atomic scale

$$\pm_{cr} = \sqrt{\frac{2¥E_H}{®r_1}} \tag{8}$$

The simplest point defect is a vacancy, which involves a missing atom (Fig. 3) within a crystal lattice. Such defects can be a result of imperfect packing during the original crystallization, or they may arise from thermal vibration of the atoms at elevated temperatures. If thermal energy is increased there is an increased probability that one afer another atoms will jump out of their position of lowest energy. Therefore, crack can propagate and diameter of vacancies may be $2a_E$,$3a_E$,...,na_E. So that the necessary condition for the critical fracture stresses may be written in the form

$$\pm_{cr}^{(n)} = \sqrt{\frac{2¥E_H}{n®r_1}} = n^{-\frac{1}{2}} \pm_{cr}, n = 1,2,3,... \tag{9}$$

In the plot of the logarithm of size, the law is a straight line (Fig. 4). The slope of this line is -1/2.

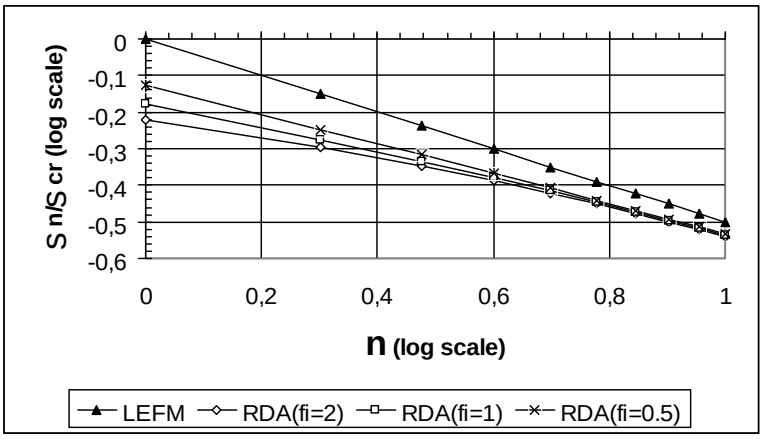

Figure 4. The size effect law of crystal lattice of iron (φ^*=2, 1 and 0.5)

The viscosity-induced size effect varies with the rates of loading and deformation and only vanishes as the rates drop to zero. For this reason the RDA size effect at the atomic scale is given by RDA fatigue limit in symmetric cycle Milašinović [3], when relative frequency $\delta \to \infty$

$$\underset{\lim ¢ \to \infty}{\pm_e}(-1) = \pm_{cr} \frac{1 + i^{¨ *}}{1 + {}^{¨ *} + i^{¨ *}} \tag{10}$$

Thus the necessary condition for the critical fracture stresses may be written in the form

$$\pm_e^{(n)}(-1) = n^{-\frac{1}{2}} \frac{1 + n^{¨ *}}{1 + {}^{¨ *} + n^{¨ *}} \pm_{cr} \tag{11}$$

This is the RDA type of scaling, where visco-elato-plasticity implies a size effect and which vanishes only when creep coefficient $\varphi^* \to 0$.

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