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Analysis of kink deformation and delamination behavior in layered ceramics

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ABSTRACT

Ceramics that are composed of layers have attracted attention because they are expected to improve the ductility. In this study, we construct a practical model of layered ceramics to deal with both interlayer slip and delamination. The deformation modes and mechanical properties under compression force parallel to the tangential direction of the layers are examined using the particle dynamics method. The effects of the stiffness of in-layer bending, the strength of the interlayer bond, and the stiffness of the elastic support associated with the surrounding materials are studied in detail, as well as the effect of strain rate. It is shown that these parameters have something to do with the criteria of kink deformation and the successive deformation mode.

1. Introduction

The development of materials that realize simultaneous increases of ductility and strength is an important topic. Conventional ceramic materials are strong in hardness and weak in brittleness with loading [1,2], whereas metals and metal alloys usually show excellent mechanical properties in ductility. Meanwhile, novel ceramics, denoted as "MAX phases," have attracted attention since the discovery of their superior mechanical properties. The properties of $M_{n+1}AX_n$ phases ("MAX phases," where $n = 1$, 2, or 3) [3–5] bridge the gap between those of typical metals and those of ceramics [6–8]. The materials have a multilayer microstructure and show some ductility for compression loads with the help of a combination of delamination and kink-band formation. The unique mechanical properties [9] of MAX phases are closely related to kink deformation processes [10–15]. For example, the reversible hysteresis in MAX phases caused by the formation, kink bands and so on has been examined [16].

In a broad sense, kink deformation in layered solids is an inelastic deformation in which a laminated surface is bent out of plane with geometrical nonlocality and nonlinearity. The deformation occurs under compression force in the direction parallel to the layers, and it is commonly observed in layered solids beyond scales such as basal slip in hexagonal close-packed metals and stratum deformation on a geological scale [17]. The deformation mechanism has been investigated in the classical literature, e.g., [18], and it is considered essential from the viewpoint of improving mechanical properties and realizing novel functionality. One reason for the generation of kink deformation in materials is crack growth, and experimental observation and theoretical analysis of fracture properties have been reported [19–21]. The geological analysis of kink banding [22] and the instability of materials which is similar with kink deformation have been explained [23]. The geometrical properties of orthokinks [24,25] and ridge-shaped kink structures [26] have been studied in metals.

Delamination is another important deformation mechanism in layered solids. Both kink deformation and delamination are commonly observed in some multilayered solids that usually show strong anisotropy due to the different structures along the transversal and stacking directions, respectively. However, such anisotropy sometimes yields surprising deformation characteristics in geometrically nonlinear deformation. Kink deformation could realize not only the improvement of deformability but also the strengthening. According to damage mechanics and fracture mechanics, the strength of materials is usually degraded by delamination. However, microcracking, which is related to the relaxation process of strain energy, may improve the toughness.

In this study, the microdynamic simulation of compression parallel to basal planes in MAX-phase ceramics is carried out using a spring–mass model based on our previous work [27]. By considering the geometrical nonlinearity of deformation, kink deformation and delamination are related to lattice rotation and debonding,

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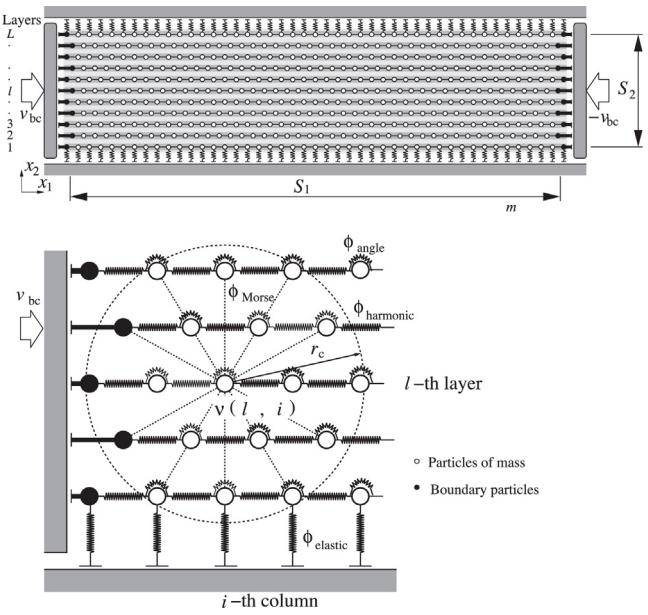

Fig. 1. Analysis model of layered solid with spring–mass model.

respectively. According to the parametric studies with stiffness of interlayer bonds and elastic support, the relationships between force–displacement curves and deformation are discussed in detail. The deformation process is related to energy release, and we expect to obtain knowledge for the improvement of toughness in the design of materials with layered microstructures.

2. Computational model

2.1. Equation of motion of the particle system

The deformation modes and mechanical properties under compression force parallel to the tangential direction of the layers are examined using the particle dynamics method.

A rectangular specimen of layered ceramics in an elastic matrix is discretized by particles with translational degrees of freedom and analyzed by the spring–mass model, as shown in Fig. 1(a). The interaction of particles is defined by a force field as a function of the configuration, which is shown in Fig. 1(b). The total number of laminating layers is L, and the lth layer ($l = 1, 2, \ldots, L$) contains $n(l)$ particles arranged in the direction of x_1 in the initial stage. The particle $\nu(l,i)$ denotes the ith particle in the lth layer, and the particle α belongs to the lamination layer, expressed by $\lambda(\alpha)$, where $l = \lambda(\nu(l, i))$ holds for any ith particle in the lth layer.

We assume a single-component material and every particle is identical. The mass of particle $\alpha(\alpha = 1, \ldots, N)$ and coordinates at time t are m.

For the simplicity, a two-dimensional model is assumed, and the equation of motion of the coordinates $\boldsymbol{x}^{[\alpha]}(t) = (x_1^{[\alpha]}(t), x_2^{[\alpha]}(t))$ of particle α is given as

$$m\frac{d^2\boldsymbol{x}^{[\alpha]}}{dt^2} = \boldsymbol{F}^{[\alpha]}, \quad (\alpha = 1, \ldots, N), \tag{1}$$

where $\boldsymbol{F}^{[\alpha]}$ is the force applied to particle α.

2.2. Force field

The force applied to a particle α is $\boldsymbol{F}^{[\alpha]} = -\partial\Phi/\partial\boldsymbol{x}^{[\alpha]}$, where the potential Φ is assumed to be expressed by

$$\Phi = \Phi_{\text{bond}} + \Phi_{\text{angle}} + \Phi_{\text{interlayer}}, \tag{2}$$

where Φ_{bond}, Φ_{angle} and $\Phi_{\text{interlayer}}$ are the potentials.

The relative position vector of particle β referred by α is $\boldsymbol{r}^{[\alpha,\beta]} = \boldsymbol{x}^{[\beta]} - \boldsymbol{x}^{[\alpha]}$, and the distance between these two particles is $r^{[\alpha,\beta]} = |\boldsymbol{r}^{[\alpha,\beta]}|$. The angle between bonds α-β and β-γ are given as

$$\theta^{[\alpha,\beta,\gamma]} = \cos^{-1}\left(\frac{(\boldsymbol{r}^{[\alpha,\beta]}, \boldsymbol{r}^{[\beta,\gamma]})}{r^{[\alpha,\beta]}r^{[\beta,\gamma]}}\right), \tag{3}$$

The potential energy of the neighboring bond in the same layer Φ_{bond} is defined by

$$\Phi_{\text{bond}} = \sum_{l=1}^{L}\sum_{i=1}^{n(L)-1}\phi_{\text{harmonic}}(r^{[\nu(l,i),\nu(l,i+1)]}). \tag{4}$$

The harmonic potential ϕ_{harmonic} is

$$\phi_{\text{harmonic}}(r) = C_{\text{pair}}(r - r_0')^2, \tag{5}$$

where C_{pair} denotes the spring constant, r is the distance between particles, and r_0' denotes a reference length.

The potential energy depending on the angle between bonds in the same layer is

$$\Phi_{\text{angle}} = \sum_{l=1}^{L}\sum_{i=1}^{n(L)-2}\phi_{\text{angle}}(\theta^{[\nu(l,i),\nu(l,i+1),\nu(l,i+2)]}), \tag{6}$$

where the potential $\phi_{\text{angle}}(\theta)$ is a function of the angles between two bonds, θ.

$$\phi_{\text{angle}}(\theta) = \begin{cases} C_\theta\dfrac{\pi^4}{972} & (\theta < -\dfrac{1}{3}\pi) \\ C_\theta\dfrac{1}{36}\theta^2(9\theta^2 + 8\pi\theta + 2\pi^2) & (-\dfrac{1}{3}\pi \le \theta < 0) \\ C_\theta\dfrac{1}{36}\theta^2(9\theta^2 - 8\pi\theta + 2\pi^2) & (0 \le \theta < \dfrac{1}{3}\pi) \\ C_\theta\dfrac{\pi^4}{972} & (\dfrac{1}{3}\pi \le \theta), \end{cases} \tag{7}$$

where C_θ is the spring constant.

The function $\phi_{\text{angle}}(\theta)$, which consists of a monotonically increasing part, $(0 < |\theta| < \frac{1}{3})$, and a plateau part, $(|\theta| \ge \frac{1}{3})$, simulates a typical grain boundary energy as a function of misorientation angle. The first derivative, $\phi'_{\text{angle}}(\theta)$, is continuous and smooth, and the second derivative, $\phi''_{\text{angle}}(\theta)$, is continuous. These features not only have good physical interpretation, they also satisfy the prerequisite for computational calculations.

The potential energy of the interlayer's interaction, $\Phi_{\text{interlayer}}$, is given by

$$\Phi_{\text{interlayer}} = \sum_{\substack{\alpha=1 \\ \lambda(\beta)\neq\lambda(\alpha)}}^{N}\sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N} R\phi_{\text{Morse}}(r^{[\alpha,\beta]}), \tag{8}$$

where the factor R is a parameter and the Morse potential, ϕ_{Morse}, between particles is defined by

$$\phi_{\text{Morse}}(r) = D\{\exp(-2\alpha(r - r_0)) - 2\exp(-\alpha(r - r_0))\}, \tag{9}$$

where D is a constant related to the binding energy, r_0 is a reference length, and α is a nondimensional parameter. A cut-off function is used for $r_1 < r < r_c$ with fixed r_1 and r_c.

Generally speaking, when the cut-off radius is large, the deformation is more strongly affected by the reference lattice configuration. Because we want to simulate some universal features of deformation which do not depend on the lattice structure, we use a short-range potential in this study.