Simulation of the Shock-Induced Phase Transition and Spall of Cerium

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Abstract.: Z-cut quartz flyer was accelerated by a power gun to impact on cerium sample to study the shock-induced $\gamma \rightarrow \alpha$ isostructural transition and spallation, The free surface velocity profile was successfully obtained with DPS technique. Two-phase equations of state for cerium were constructed based on first-principles calculations. A previous dynamic micro-void nucleation and growth model and a newly-proposed phenomenal phase transition model were applied to simulate the experiments, the simulated free surface velocity profiles agree with experimental lines very well

1. Introduction

As the first of the rare earth elements Cerium displays intriguing physical and chemical properties of which the most fascinating is its first-order isostructural $\gamma \rightarrow \alpha$ phase transition at about 298 K and 0.7 GPa[1]. The transition are accompanied by a lost of the magnetism and a giant volume collapse (~17%)[2] leaving the crystal structure unchanged as face-centered cubic (fcc). A great number of experimental and theoretical efforts have been devoted to investigate the phase diagram and explore the underlying physics governing the volume collapse whose size decreases with increasing temperature and eventually terminates in a critical point (CP)[3-8]. In this paper we are interested in the shock-induced $\gamma \rightarrow \alpha$ transition and the spallation. First, plate impact experiments were performed, after that two-phase equations of state (EOS) were constructed based on first-principles calculations, and a previous dynamic micro-void nucleation and growth model and a newly-proposed phenomenal phase transition model were applied to simulate the experiments. The simulated free surface velocity profiles agree with experimental lines well.

2. Experiments

The schematic experimental configuration is shown in Fig.1. The *z*-cut α-quartz single crystal flyer was accelerated by a power gun to impact on the cerium sample, two DPS probes[9] were used to measure the impact velocity and the sample's free-surface velocity, respectively. The flyer was 7.5 mm in thickness, and the sample 1.5 mm. One-dimension strain condition has already been considered. Two shots have been carried out, the impact velocities were measured 197.3 m/s and 247.6 m/s, respectively. The free-surface velocity profiles were shown in Fig.2.

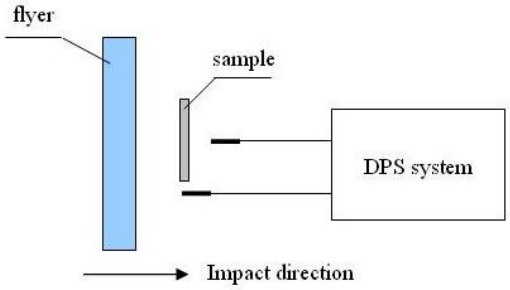

Fig.1 The schematic experimental configuration

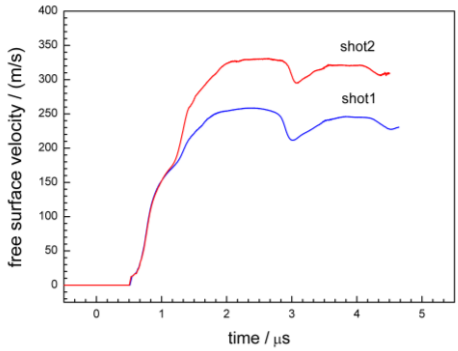

Fig.2 The experimental free-surface velocity profiles

3. Two-phase Equations of State

We formulated the EOS by evaluating the Helmholtz free energies of both phases as functions of temperature and specific volume. The free energy was generally expressed as

$$F(V,T) = E_C(V) + F_{ion}(V,T) + F_e(V,T) + F_{mag}(V,T) \tag{1}$$

Where $E_C(V)$ is the static cohesive energy with all atoms fixed at their ideal crystal positions, $F_{ion}(V,T)$ denotes the lattice vibrational free energy, $F_e(V,T)$ is the contribution due to thermal excitation of electrons from their ground state, $F_{mag}(V,T)$ is the magnetic free energy, this term is only for γ phase. $F_{ion}(V,T)$ was constructed in the form

$$F_{ion}(V,T) = \frac{9}{8}NK_B\Theta(V) + 3NK_BT\ln\left[\left(1-e^{-\Theta(V)/T}\right)(1+\beta T)^{1/2}\right] - NK_BTD\left(\frac{\Theta(V)}{T}\right) \tag{2}$$

Eq.(2) is modified from Debye model, in which $\Theta(V)$ is the volume-dependent Debye temperature calculated by following equations

$$\Theta(V) = \frac{h\nu_m(V)}{K_B} \tag{3}$$

$$\frac{\partial \ln \nu_m(V)}{\partial \ln V} = -\gamma_{ion}(V) \tag{4}$$

$$\gamma_{ion}(V) = \left(\frac{\alpha}{2} - \frac{2}{3}\right) - \frac{V}{2}\frac{f''(V)}{f'(V)} \tag{5}$$

$$f(V) = P_C(V)V^{\alpha} \tag{6}$$

$\gamma_{ion}(V)$ is the Grüneisen parameter, α takes the value 3/4 according to free volume theory[10]. $P_C(V)$ is the cold pressure. The Debye integration in eq.(2) is expressed as

$$D(z) = \frac{3}{Z^3}\int_0^Z dx \frac{x^3}{e^x - 1} \tag{7}$$

The parameter β in Eq.(2) was introduced by Кормер to descript the strong anharmonic effects of lattice[see Ref.11]. The other terms in Eq.(1) were directly calculated from first-principles with DFT+U method. The details of EOS calculations will be published in other place. In Fig.3 the phase diagram computed from our EOS was compared with experimental data showing good agreement.

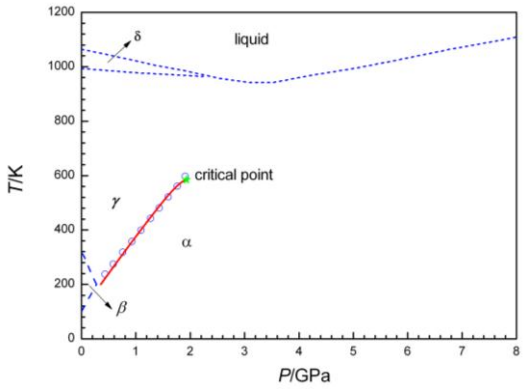

Fig.3 Phase diagram of Cerium (Cycles are of experiments, solid is calculated line)

4. Phenomena models for phase transition and spall

Simulations in the present work used a homogeneous mixture model for phase transition

similar to Duvall and Graham[12]. However the rate of change of mass fraction was calculated according to following consideration.

Using η , Gmother and Gdaughter to denote the mass fraction of mother phase, the Gibbs free energy of mother and daughter phases, respectively, and a dot signal on each variable represents its time derivative, first derive an express for $\dot{\eta}$ under the assumption $\dot{G}_{mother} = \dot{G}_{daughter}$, we call this express $\dot{\eta}_{balance}$, then the real express for $\dot{\eta}$ used in simulations is formulated as

$$\dot{\eta} = \exp(a \cdot \frac{G_{\text{mother}} - G_{\text{daughter}}}{T}) * \tanh[b \cdot (c - \eta)] \cdot \dot{\eta}_{balance} \tag{8}$$

Where a, b, c are model parameters determined by fitting the theoretical free surface velocity profile to the experimental curve.

A previous model proposed by authors was applied to simulate the spall behavior of samples. The variable for damage was defined as the fraction of void volume, $D = V_V / V$, V_V is void volume, V the total volume. The evolution of D was derived in an energy balance approach.

$$\begin{aligned} \dot{D} = & \left\{ \begin{array}{lll} \frac{4\pi}{3} R_{\text{N}}^3 \rho N_0 \exp(\frac{P_{\text{m}} - P_0}{P_1}), & -P_{\text{m}} \geq P_0 \quad \text{and} & D < D_0 \\ 0, & -P_{\text{m}} < P_0 \quad \text{or} & D \geq D_0 \end{array} \right\} \\ & + \left\{ \begin{array}{ll} \frac{3C_{\text{b}}}{4B_{\text{m}}\lambda} (P_{\text{m}}^2 - \sigma_0^2) D(1-D), & -P_{\text{m}} \geq \sigma_0 \\ 0, & -P_{\text{m}} < \sigma_0 \end{array} \right\} - D\dot{\varepsilon}_{\text{b}} \end{aligned} \tag{9}$$

As the physical meanings of the variables in Eq.(5), please refer to authors' paper [13]

The shear strength and the bulk modulus of damaged material were calculated by modified Mackenzie formulas[14]

$$G_D = G_0(1-D)\left(1 - D\frac{6B_0 + 12G_0}{9B_0 + 8G_0}\right)F(D) \tag{10}$$

$$B_D = \frac{4G_0 B_0 (1-D)}{4G_0 + 3B_0 D} F(D) \tag{11}$$

$$F(D) = \exp\left[-\left(\frac{D}{D_1}\right)^{\alpha}\right] \tag{12}$$

The term $F(D)$ was introduced by authors to describe the rapid relaxation of stress when voids come to near coalescence[13]. In above equations, G_0 and B_0 are the shear and bulk moduli of the undamaged material, D_1 and α are model parameters.

5. Simulation Results

In the present simulations, the constitutive relation of cerium sample was dealt with ideal elastic-plastic model. The yielding stress was set 80 MPa. Within the experimental pressure arrange, z-cut quartz was found to respond to shock loadings linear elastically. Its stress-volume curve had been measured high precisely, the result please refer to our reference [9]. The details of the simulations will be published in other place, in Fig.4 the calculated free surface velocity profiles are compared to experimental data, we can see they are in good agreement.

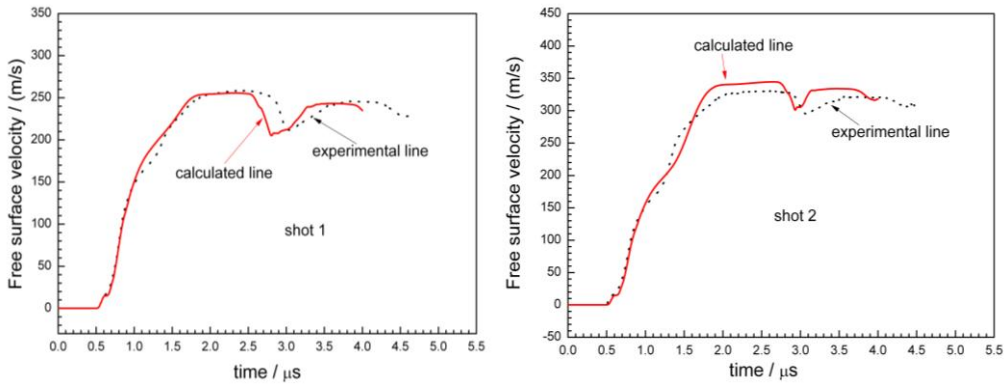

Fig.4 Simulated free surface velocity profiles

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