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Inhomogeneous strain fields within silicon spheres under the point load test and the strain effect on the quantum valence-bands

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A B S T R A C T

This paper presents an exact solution for inhomogeneous strain and stress distributions within silicon spheres under the point load test. The contact problem between the spherical head of the steel cones and the surfaces of the silicon spheres is considered. Displacement functions are introduced in order to uncouple the governing equations. The Fourier–Legendre expansion technique is employed so that all of the boundary conditions can be satisfied exactly. When the isotropic limit is considered, the classical solution by Hiramatsu and Oka [20] is covered as a special case. It was found that the strain distributions are relatively uniform within central part (say $r/R<0.6$, where r and R are the distance from the center and the radius of the sphere, respectively) of the silicon spheres under the point load test, but very high tensile strain concentrations are usually developed near $r/R=0.9$. In addition, based on quantum mechanics and energy band theory, the effect of strain on three quantum valence-bands of silicon is analyzed. Numerical results show that the large strain induced at $r/R=0.9$ of the sphere under the point load test significantly breaks some symmetric property of quantum valence bands of silicon, and has obvious effect on the constant energy surfaces and the conductivity effective masses of heavy hole (HH) band, the light hole (LH) band and the split-off (SO) band, which is closely related to optical and electric property of silicon.

1. Introduction

The performance improvement of the complementary metal oxide semiconductor (CMOS) circuits has become extremely difficult due to short channel effects of the conventional bulk silicon [1,2]. However, there is increasing interest in employing strained silicon, since strain can brake the inversion symmetry of the electronic structure of silicon, thus improving significantly the mobility of charge carriers [3]. For example, it was found that strain is the key technique for 45 nm CMOS [4], and makes it possible to use strained silicon as a new kind of electro-optic materials [5]. Biaxial tensely strained silicon is used as a channel in metal oxide semiconductor field effect transistor because of electrons and holes mobility enhancement induced by strain [6]. Advanced CMOS imaging systems can gain in resolution and speed by using strained silicon [7]. Very fast flexible electronics needed in macroelectronics and radio frequency identification require unique property significantly enhanced by strained silicon [8]. It has been demonstrated that high levels of tensile strain in silicon can be induced by the fabrication of silicon nanomembranes [9].

The sensitive dependence of carrier mobility on strain makes the quantitative measurement of strain, its distribution, and its effect on the band structure of silicon highly desirable [10,11]. Peng et al. [12] observed significant change in band gap with nonhydrostatic strains. Shiri et al. [13] studied the uniaxial strain effects on band gap and effective mass. Kalenci et al. [14] investigated the local strain distributions in silicon-on-insulator/stressor-film composites. Saxena and Kumar [15] designed a new strained-silicon channel for metal-oxide-semiconductor field-effect transistor (MOSFET). Wei [16] shows that the stress and strain distribution within finite cylinders under compression test are inhomogeneous as long as friction exists, and friction has considerable effect on valence band structure, which is manifested as changes in band splitting, and alteration of the shape of constant energy surfaces of the heavy-hole and the light-hole bands. Moreover, high stress level is usually needed to significantly improve the hole mobility of silicon. The highest local stress induced is up to 4 GPa [17]. Therefore, it is very important to generate high local stresses in silicon. Wei et al. [18] obtained an analytical solution for inhomogeneous strain within cylinders of silicon and analyzed the effect on quantum band structure under the double-punch test. It is found that double-punch test

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can change considerably the valence band of silicon, and the effect is even much more significant than a cylinder under uniaxial test.

All of the analysis are for cylinders under various boundary conditions. Spheres under the point load test, which is one of the popular indirect tensile strength test for brittle materials, have also been studied. More specifically, Sternberg and Rosenthal [19] employed the Boussinesq stress function in dipolar coordinates and obtained the first solution for isotropic spheres under concentrated diametrical loads. Hiramatsu and Oka [20] derived an analytical solution for isotropic spheres under diametrical point loads. Chau and Wei [21] derived an analytical solution for stress concentrations within a spherically isotropic sphere under point loads. Wei [22] analyzed the stress and strain distributions of spheres of $Si_{1-x}Ge_x$ alloy under compression between two flat platens. However, there is no analysis for the strain distributions or the effect on the quantum behavior of electronic structure of silicon spheres under the point load test.

In this paper, the inhomogeneous strain distribution within solid spheres of silicon under the point load test is studied. Displacement functions are introduced in order to uncouple the governing equations, and the displacement functions are further expressed in terms of Legendre functions so that a closed-form solution can be obtained. In addition, based on quantum mechanics and energy band theory, the effect of strain on the quantum valence band structure of sphere of silicon under the point loads is studied.

2. Governing equations

Consider a spherical polar coordinate system (r,θ,φ) with the origin locating at the center of silicon sphere as shown in Fig. 1. Experimental results show that silicon is a kind of cubic isotropic material [23], so the generalized Hooke's law for a silicon sphere can be written as

$$\begin{aligned}&\sigma_{rr}=c_{11}\varepsilon_{rr}+c_{12}\varepsilon_{\theta\theta}+c_{12}\varepsilon_{\varphi\varphi},\quad \sigma_{\theta\theta}=c_{12}\varepsilon_{rr}+c_{11}\varepsilon_{\theta\theta}+c_{12}\varepsilon_{\varphi\varphi}\\&\sigma_{\varphi\varphi}=c_{12}\varepsilon_{rr}+c_{12}\varepsilon_{\theta\theta}+c_{11}\varepsilon_{\varphi\varphi},\ \ \sigma_{r\theta}=2c_{44}\varepsilon_{r\theta},\ \ \sigma_{\theta\varphi}=2c_{44}\varepsilon_{\theta\varphi},\ \ \sigma_{r\varphi}=2c_{44}\varepsilon_{r\varphi}\end{aligned}\tag{1}$$

where the Cauchy stress tensor is denoted by σ and the strain tensor by ε. c_{11}, c_{12} and c_{44} are three independent elastic constants of the silicon.

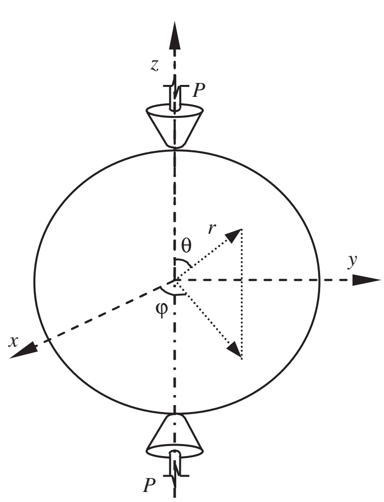

Fig. 1. A silicon sphere under the point load test.

For the present problem of spheres under point load test, body forces can be neglected. The equations of equilibrium are:

$$\begin{aligned}&\frac{\partial\sigma_{rr}}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial\sigma_{r\varphi}}{\partial\varphi}+\frac{1}{r}\frac{\partial\sigma_{r\theta}}{\partial\theta}+\frac{2\sigma_{rr}-\sigma_{\theta\theta}-\sigma_{\varphi\varphi}+\sigma_{r\theta}\cot\theta}{r}=0\\&\frac{\partial\sigma_{r\varphi}}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial\sigma_{\varphi\varphi}}{\partial\varphi}+\frac{1}{r}\frac{\partial\sigma_{\theta\varphi}}{\partial\theta}+\frac{3\sigma_{r\varphi}+2\sigma_{\theta\varphi}\cot\theta}{r}=0\\&\frac{\partial\sigma_{r\theta}}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial\sigma_{\theta\varphi}}{\partial\varphi}+\frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta}+\frac{3\sigma_{r\theta}+(\sigma_{\theta\theta}-\sigma_{\varphi\varphi})\cot\theta}{r}=0\end{aligned}\tag{2}$$

The relations between the strain and displacement components in spherical polar coordinate are:

$$\begin{aligned}&\varepsilon_{rr}=\frac{\partial u_r}{\partial r},\quad \varepsilon_{\theta\theta}=\frac{1}{r}\frac{\partial u_\theta}{\partial\theta}+\frac{u_r}{r},\quad \varepsilon_{\varphi\varphi}=\frac{1}{r\sin\theta}\frac{\partial u_\varphi}{\partial\varphi}+\frac{u_r}{r}+\frac{u_\theta}{r}\cot\theta\\&\varepsilon_{r\varphi}=\frac{1}{2}\left(\frac{1}{r\sin\theta}\frac{\partial u_r}{\partial\varphi}-\frac{u_\varphi}{r}+\frac{\partial u_\varphi}{\partial r}\right),\quad \varepsilon_{r\theta}=\frac{1}{2}\left(\frac{1}{r}\frac{\partial u_r}{\partial\theta}-\frac{u_\theta}{r}+\frac{\partial u_\theta}{\partial r}\right)\\&\varepsilon_{\theta\varphi}=\frac{1}{2}\left(\frac{1}{r}\frac{\partial u_\varphi}{\partial\theta}-\frac{u_\varphi}{r}\cot\theta+\frac{1}{r\sin\theta}\frac{\partial u_\theta}{\partial\varphi}\right)\end{aligned}\tag{3}$$

where u_θ, u_φ and u_r are displacements in θ, φ and r directions, respectively.

3. Boundary conditions for silicon spheres under the point load test

In the point load test, the point loads with magnitude F are usually applied on a sphere of radius R through a pair of steel cones with spherical heads (Fig. 1). Since the contact is usually developed between the spherical heads and the spherical specimen, the contact stress can be obtained by considering the contact problem between two spheres [24], and all other tractions on the surface of the sphere are zero. Therefore, the boundary condition for a silicon sphere under the point load test can be expressed as

$$\sigma_{rr}=\begin{cases}-p(\theta) & \text{for } 0\le\theta\le\theta_0 \text{ and } \pi-\theta_0\le\theta\le\pi\\ 0 & \text{for } \theta_0<\theta<\pi-\theta_0\end{cases}\tag{4}$$

$$\sigma_{r\varphi}=\sigma_{r\theta}=0\tag{5}$$

on $r=R$, where

$$p(\theta)=\frac{p_0R}{R_0}\sqrt{\cos^2\theta-1+\left(\frac{R_0}{R}\right)^2}\tag{6}$$

$$p_0=\frac{3F}{2\pi{R_0}^2}\tag{7}$$

$$R_0=\left[\left(\frac{1-v^2}{\pi E}+\frac{1-v_2^2}{\pi E_2}\right)\frac{3\pi FR_2R}{4(R+R_2)}\right]^{1/3}\tag{8}$$

where R is the radius of the sphere, F is the magnitude of the applied point force, R_0 is the radius of the circular contact area, and R_2, E_2 and v_2 are the radius of the spherical heads, Young's modulus and Poisson's ratio of the steel cones, respectively. According to the requirement for the standard point load test, the spherical head is made of tungsten carbide [21]. Thus, Young's modulus E_2 can be assumed to be large enough such that $(1-v_2^2)/\pi E_2\to 0$ can be used in Eq. (8).

Now our problem is to obtain solutions satisfying the fifteen governing equations (1)–(3) and boundary conditions (4) and (5). The method of solution is to be presented next.