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Solution for the critical thickness models of dislocation generation in epitaxial thin films using the Lambert *W* function

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Abstract An exact analytical solution for the equilibrium critical thickness of misfit dislocation generation in epitaxial thins films is presented. The new expression is based on the use of the Lambert *W* function which eliminates the need of complex iterative computation. The comparison of proposed analytical solution versus misfit strain with the equilibrium critical thickness based on numerical solution proves its high accuracy.

Introduction

Since 1987, Freund [1] introduced a theoretical approach to calculate the critical film thickness of dislocation generation in epitaxial thin films. This approach based on the criterion stability of dislocation represents an elasticity theory approach. In its general form, this model is very similar to the more familiar equilibrium approach summarized by Matthews and Blakeslee [2] based on the force equilibrium criterion. However, the model was deficient insofar as it does not provide an explicit expression for the equilibrium critical thickness h_c. The implicit expression was presented as:

$$h_c = A\left[\ln\left(\frac{2h_c}{r_0}\right) - B\right], \tag{1}$$

where A, B, and r_0 represent the material constants.

Equation 1 can be solved numerically by an iterative method. This is not necessary; the exact solution of this equation is given by the so-called Lambert *W* function [3]. This function was postulated to solve the equation:

$$W(z)\exp W(z) = z. \tag{2}$$

The Lambert *W* function allows the explicit solution of entire classes of differential equations, which previously could only be solved numerically, and is today experiencing a renaissance in various fields of sciences and engineering [4–6].

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Results and discussion

The existence of a critical thickness for dislocation generation in thin films was first proposed by Frank and Van der Merwe [7] and it was subsequently confirmed experimentally. Indeed, if the misfit strain between the substrate material and the film material is sufficiently small, or when the film is very thin, it can be accommodated elastically. However, as the film thickens, the energy required for elastic accommodation increases and eventually becomes excessive, and the dislocations are generated as an alternative means to accommodate the misfit.

Two approaches are generally followed in the theoretical studies of critical thickness of strained epitaxial films. The first approach involves the comparison of the Gibbs free energy of the two strained systems, with and without the misfit dislocation. The second approach considers the balance between two driving forces, one originating from the misfit strain that tends to lengthen the misfit dislocation, and the other from the line tension that tends to shorten it. Noting that the two approaches are not independent of each other and, indeed, Freund [1] and Nix [8] showed that the two approaches lead to precisely the same results.

The two approaches have been discussed in many works [9, 10] and the investigations of the critical thickness based on either one of the foregoing approaches have been reported in the literature. Thus, Matthews and Blakeslee [2] derived an equation for the critical thickness by assuming a critical balance between the force generated by the lattice mismatch on a segment of a propagating threading dislocation, and the extra line tension associated with a newly created interfacial dislocation. Freund [1] systematically investigated the driving force for glide of a threading dislocation. The equation for the equilibrium critical thickness as obtained by Freund's [1] analysis is given by:

$$h_c = \frac{b}{8\pi(1+v)\varepsilon_0 \sin\alpha}\left\{\ln\left(\frac{2h_c}{r_0}\right) - \frac{1}{2}\cos 2\alpha - \frac{(1-2v)}{4(1-v)}\right\}, \tag{3}$$

where b is the magnitude of the Burgers vectors, v is the Poisson ratio of the epilayer material, ε_0 is the misfit strain, r_0 is the cut-off radius for the dislocation core, and α is the angle between the glide plane and interface. Equation 3 can be solved exactly, using the approach proposed by Braun et al. [11].

For further calculation, we introduce the abbreviations

$$A = \frac{b}{8\,\pi(1+v)\varepsilon_0 \sin\alpha} \tag{4}$$

$$B = \frac{1}{2}\cos 2\alpha + \frac{(1-2v)}{4(1-v)} \tag{5}$$

and

$$z = -\frac{r_0}{2A}\exp(B) \tag{6}$$

Using the transformation $h_c \to u = \frac{2h_c}{r_0}$, we obtain the simple implicit equation:

$$\frac{r_0}{2A}u - \ln(u) = -B \tag{7}$$

For solving Eq. 7 we suppose that:

$$u = \exp(B)\frac{W(z)}{z} \tag{8}$$

Inserting Eq. 8 into Eq. 7 yields

$$W(z) + \ln\left(\frac{W(z)}{z}\right) = 0 \tag{9}$$

Rearranging Eq. 9 and employing an exponential in Eq. 11

$$W(z) + \ln(W(z)) - \ln(z) = 0 \tag{10}$$

$$\exp(W(z) + \ln(W(z)) - \ln(z)) = 1 \tag{11}$$

$$W(z)\exp W(z) = z \tag{12}$$

We find that Eq. 12 represent the definition of the Lambert W function, as already established in Eq. 2.

Consequently, our hypothesis in Eq. 8 is justified.

The exact solution for the equilibrium critical thickness is after resubstitution for z

$$h_c = -A\,W\left(-\frac{r_0}{2A}\exp(B)\right) \tag{13}$$

And after replacing A and B

$$h_c = -\frac{b}{8\pi(1+v)\varepsilon_0 \sin\alpha} \times W\left(\frac{-r_0}{2A} \times \exp\left(\frac{1}{2}\cos 2\alpha + \frac{(1-2v)}{4(1-v)}\right)\right) \tag{14}$$

The Lambert W function is a complex and multivalued function with an infinite number of branches, only two of them having real values. If x is real, then for $-\frac{1}{e} \le x \le 0$, there are two possible real values of $W(x)$, as displayed in Fig. 1. The branch satisfying $-1 \le W(x)$ is denoted $W_0(x)$ and referred to as the principal branch in the literature [12]; the branch satisfying $W(x) \le -1$ is denoted $W_{-1}(x)$.

We mentioned that the series representation for the Lambert W function is:

$$W(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1} z^n}{n!} \quad \text{for } |z| < \frac{1}{e} \tag{15}$$

The Lambert W function can be differentiated

$$W'(z) = \frac{W(z)}{z(1+W(z))} \quad \text{for } z \neq 0 \tag{16}$$

and also integrated

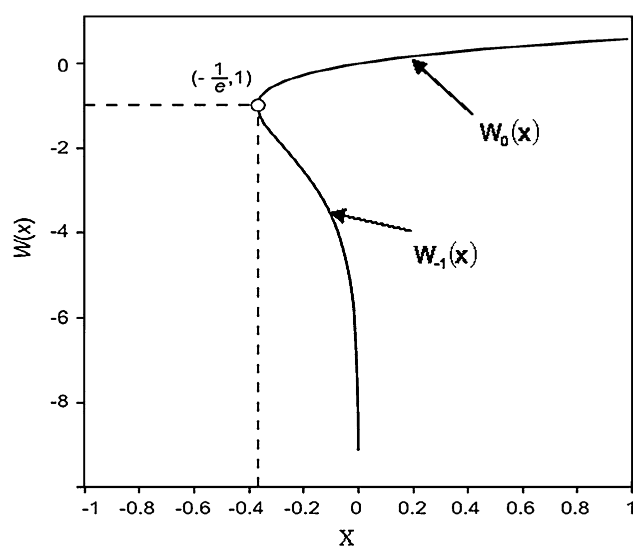

Fig. 1 Plots of real valued branches of Lambert function $W_0(x)$ and $W_{-1}(x)$

$$\int W(z)\mathrm{d}z = z\left(W(z) - 1 + \frac{1}{W(z)}\right) = \left(W(z)^2 - W(z) + 1\right) e^{W(z)} \tag{17}$$

For practical application, to find the branch of $W(x)$ that correctly describe the evolution of the critical thickness, additional reasonableness considerations are required. The equilibrium critical thickness h_c is always positive, as expected. Therefore, the argument of the Lambert W function as well as the pre-factor always has the same sign, either negative or positive. We identify $W_{-1}(x)$ (Fig. 1) as the branch that appropriately describes the evolution of the critical thickness as a function of misfit strain ε_0.

Consider the equilibrium critical thickness of $Si_{1-x}Ge_x$ thin films when growing it on a single crystal Si(001). The lattice parameter of $Si_{1-x}Ge_x$:

$$a(x) = x\,a_{\mathrm{Ge}} + (1-x)a_{\mathrm{Si}} \tag{18}$$

The misfit strain ε_0 is defined as:

$$\varepsilon_0 = \frac{a(x) - a_{\mathrm{Si}}}{a_{\mathrm{Si}}} = 0.042x \tag{19}$$

Using the material constants for SiGe with $b = r_0 = 3.84$ Å, $\nu = 0.36$, the equilibrium critical thickness of $Si_{1-x}Ge_x$ alloy as a function of the misfit strain ε_0 is shown in Fig. 2 for an example of angle $\alpha = \frac{\pi}{6}$.

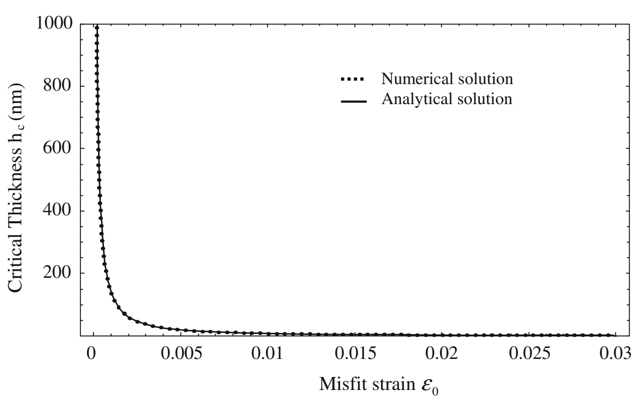

Fig. 2 Critical thickness h_c of SiGe alloy as a function of misfit strain ε_0. The *dashed curve* gives the equilibrium critical thickness as calculated from numerical solution. The *solid curve* gives the present result with $\alpha = \frac{\pi}{6}$

Comparison of the calculated equilibrium critical thickness versus misfit strain with the respective numerical solution is shown in Fig. 2. It is easily seen that good agreement is achieved for all values of misfit strain.

Conclusion

In this paper, an exact analytical solution is given for the equilibrium critical thickness of misfit dislocation generation in epitaxial thin films. Based on this new expression, no needs are necessary for complex iterative computation. The comparison with numerical results shows good agreement of the proposed solution.

Practically, this equilibrium critical thickness is easy to compute since the Lambert W function is readily available in standard computational packages. Furthermore, this mathematical approach described here can be applied to all common models for the equilibrium critical thickness, and not just for the model of Freund.

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