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IMAGE FORCES ON SCREW DISLOCATIONS IN MULTILAYER STRUCTURES

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Introduction

The study of dislocations in multilayered structures is important as a means of understanding the mechanical properties of composites and thin films. The elastic interaction of dislocations in such structures is significantly affected by the proximity of phases with different elastic properties. Image methods provide one technique of determining such interactions.

Image solutions have been obtained for a number of simple cases of straight screw dislocations parallel to the interfaces of multilayer structures (1-6). These have included the cases of a two layer freebody (4), a layer bounded by two semi-infinite bodies (3) and single, double and triple layers adjoining the free surface of a semi-infinite body (6). Koehler (5) has studied the problem of a screw dislocation in a composite material of alternating layers of two phases, but in the approximation that only the first order images contribute to the interaction.

In the present work, we have used the image method to calculate the force on an infinite and straight screw dislocation with its axis parallel to the interfaces in a multilayered structure, having alternate layers of A and B of equal thickness (h) encased in two semi-infinite layers. The treatment is extended to five layers to indicate the degree of accuracy in using the simple three layer result (3) to approximate the n-multilayer case.

Formulation

The layer phases are assumed to be elastically isotropic. The geometry of the multilayer system is shown in Fig. 1. The screw dislocation is at $x' = a$ in a five layer system. For the four layer case, interface 1 is at $x' = -\infty$, while in addition for the three layer case, interface 4 is at $x' = \infty$. The z' coordinate, parallel to the dislocation line, points out of the page.

As indicated in Fig. 2, the image situation at an interface can be represented by an analog of semireflecting mirrors. The strengths of the images can be expressed in terms of the factor $\gamma = (\mu_B - \mu_A)/(\mu_B + \mu_A)$ where μ is the shear modulus. For a dislocation at $x' = a$, the first order images correspond to a reflection with magnitude γ at interface 3 and a transmission with magnitude $(1 - \gamma)$. The higher order images represented by the dashed lines correspond to reflections with magnitude $-\gamma$ and transmissions of magnitude $(1 + \gamma)$. In other words transmission from A to B or B to A, respectively,

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modifies the magnitude of the dislocation Burgers vector or strain field by $(1-\gamma)$ or $(1+\gamma)$ while reflection in A or in B, respectively, modifies it by γ or $-\gamma$. The multiple image problem then becomes a combinatorial problem of counting reflections and transmissions for a given image path length.

For the total image force on the dislocation, the image stress σ_{yz} at $x' = a$ is required,

$$F_x/L = \sigma_{yz} b \qquad [1]$$

In order to represent the results compactly, the reduced coordinates $x = x'/h$ and $\alpha = a/h$ are convenient. In the reduced coordinates the stress appropriate for the Peach-Koehler image force is

$$\sigma_{yz}(x' = a) = \frac{\mu (b/h) \phi}{4\pi} \qquad [2]$$

where ϕ is the appropriate sum for the multilayer case. For the simple bicrystal with a single image, $\phi = 1/(a/h) = 1/\alpha$, for the three layer case, B A B in Fig. 1, the result, confirming the work of Chou (3), is $\phi = \phi_1$ with

$$\phi_1 = (1 - 2\alpha) \sum_{n=1}^{\infty} \frac{\gamma^{2n-1}}{(n + \alpha - 1)(n - \alpha)} \qquad [3]$$

for the four layer case, B A B A with interfaces 2, 3, 4 in Fig. 1, the result is $\phi = \phi_1 + \phi_2$ with

$$\phi_2 = \sum_{n=2j+m-1}^{\infty} \sum_{m=1}^{j+1} \sum_{j=1}^{\infty} \frac{(n-j)!\, j!\, (-1)^{j+1} (1-\gamma^2)^j (-\gamma)^{2n-2j-1}}{(n-2j-m+1)!\,(m-1)!\,(j-m+1)!\,(j+m-1)!} f_2(\alpha) \qquad [4]$$

$$\text{with } f_2(\alpha) = [1/(\alpha - n)] - [\gamma^2/(\alpha + n)] \qquad [5]$$

The sum in equation [4] represents all of the reflections/ transmissions in Fig. 2 exclusive of the multiple single reflections already counted in equation [2]. In the sum, j is the number of transmissions of the type shown in Fig. 2 and $1 \leqslant m \leqslant j + 1$ represents the m^{th} term in the j^{th} sum. The correspomding four layer case A B A B with interfaces 1, 2 and 3 in Fig. 1 is given by $\phi = \phi_1 + \phi_3$ with ϕ_3 of the same form as equation [4] but with

$$f_3(\alpha) = [1/(n + \alpha - 1)] - [\gamma^2/(n + 1 - \alpha)] \qquad [6]$$

for the five layer case A B A B A in Fig. 1, the result is

$$\phi = \phi_1 + \phi_2 + \phi_3 + \phi_4$$

ϕ_4 represents the sum of the images for which there is an A B transmission across both interfaces 2 and 3. A simple recursion formula could not be found for this case, but terms up to n = 14 were calculated and were found to give a convergent result for small $|\gamma|$.

In principle one can extend this type of solution to include any number of layers, but as the number of layers increase, obtaining an explicit solution becomes extremely laborious and time consuming. Hence the work was not extended beyond the five layer case.

Results and Discussion

Calculations based on the results of the image analysis were performed for several values of γ. It was found that the sums for the three layer and four layer cases converged for all values of γ, whereas the sum for for the five layer case converged only for $|\gamma| \leqslant 0.5$, that is when the ratio of the stiffer to the more pliable shear modulus is less than three. However, this is not a serious limitation as in most practical cases, the shear modulii of the two constituents of a composite material rarely differ by more than a factor of two.

The calculated image force as a function of normalized dislocation position ($\alpha = a/h$) is plotted in Figs. 3 and 4 for two γ values for the three, four and five layer cases. The magnitude of the image force is seen to increase as the value of γ increases. The results indicate that in most practical cases, the three layer solution can be used with a reasonable degree of accuracy. Tables 1 and 2 show the deviation of the four and five layer cases from the three layer case. The four layer case deviates from the three layer case more than does the five layer case because of the asymmetry of the four layer configuration. However as also shown in Figs. 3 and 4, the multiple images are important as even for small α , the deviation from the single image bicrystal result is seen to be appreciable.

Thus the implications of the results are that in calculations of dislocation forces and energies arising from elastic inhomogeneity, a good approximation can be achieved using the easily computed result of equation [2]. Hence, the extension of dislocation and crack injection problems for strained multilayers to include the elastic inhomogeneity effect in addition to coherency strains is readily achievable. Another application of the results is to determine pileup stress concentrations for layered structures. Such work is underway as well as the extension of the calculations to the edge dislocation case, which is not as tractable as the screw case.

Acknowledgement

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References

1. G. Leibfried and H. D. Z. Dietze, Z. Phys. 126, 290 (1949).
2. A. K. Head, Phil. Mag. 44, 92 (1953).
3. Y. T. Chou, Phys. Stat. Sol. 17, 509 (1966).
4. S. N. G. Chu, J. App. Phys. 53, 3019 (1982).
5. J. S. Koehler, Phys. Rev. B 2, 547 (1970).
6. M. L. Ovecoglu, M. F. Doerner and W. D. Nix, Acta Met, In press.

Table 1

Values of image force factor ϕ for $\gamma = 0.1$ together with the percent deviation from the three layer case

	Three layer	Four layer		Five layer	
α	ϕ	ϕ	% dev.	ϕ	% dev.
0.01	9.8995	9.9495	0.51	9.8507	0.49
0.10	0.88927	0.94168	5.89	0.85101	3.80
0.20	0.37528	0.43063	14.75	0.34751	7.39
0.30	0.19066	0.24930	30.75	0.17256	9.49
0.40	0.08342	0.14576	74.71	0.07449	10.70
0.50	0.00000	0.066513	_	0.12×10^{-6}	_

Table 2

Values of image force factor ϕ for $\gamma = 0.5$ together with the percent deviation from the three layer case

	Three layer	Four layer		Five layer	
a	ϕ	ϕ	% dev.	ϕ	% dev.
0.01	49.562	49.779	0.44	49.326	0.48
0.10	4.4970	4.7292	5.16	4.3114	4.13
0.20	1.9132	2.1628	13.05	1.7778	7.07
0.30	0.97732	1.2458	27.46	0.88885	9.05
0.40	0.42898	0.71787	67.34	0.38526	10.19
0.50	0.00000	0.31136	_	0.65×10^{-6}	_

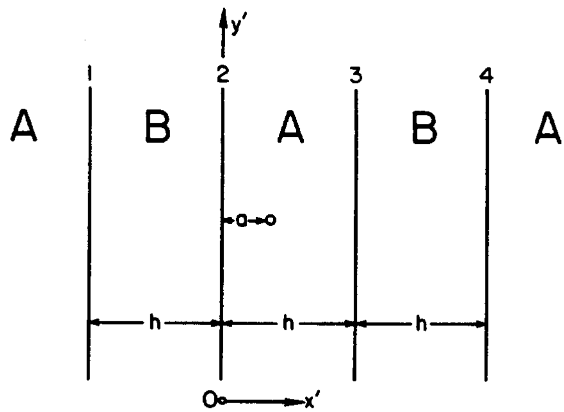

Fig. 1 Geometry of multilayer system

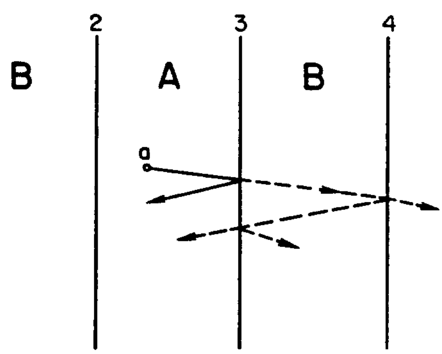

Fig. 2 Image reflections and transmissions at the interfaces

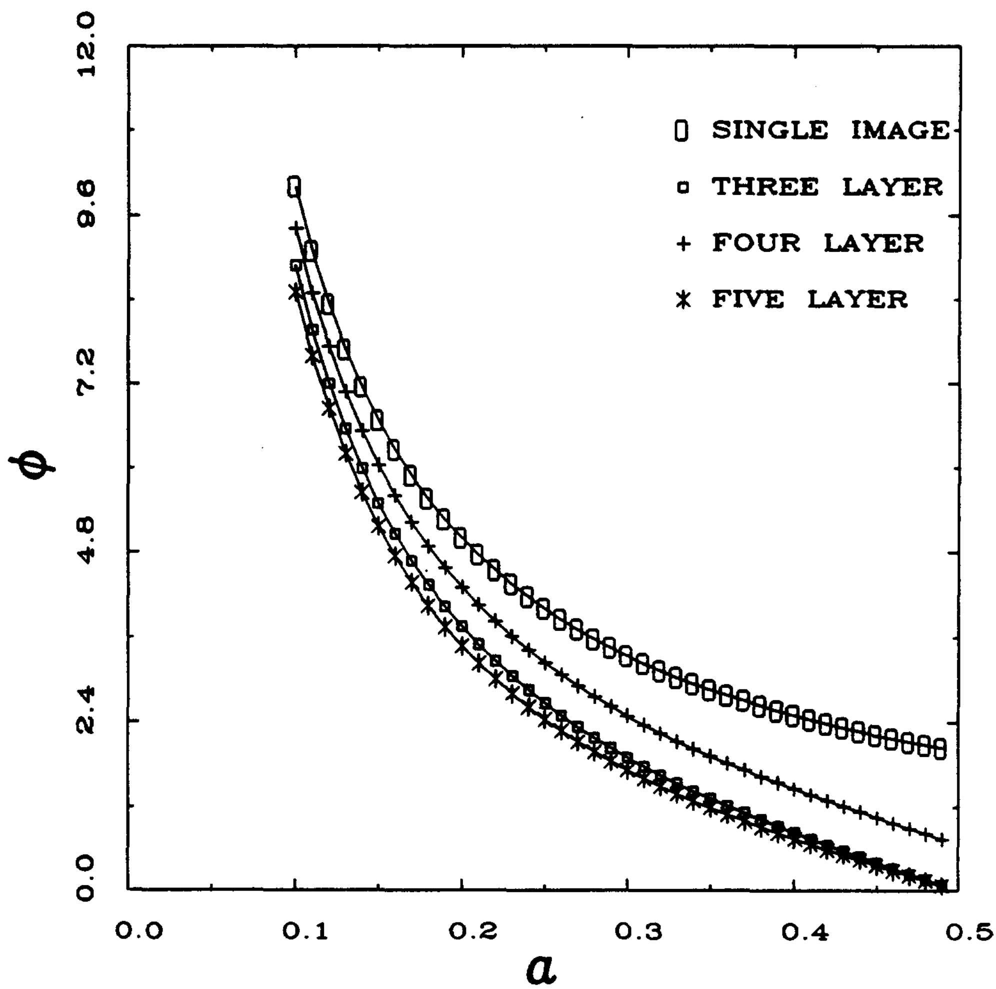

Fig. 3 Image force factor ϕ as a function of position a for three, four and five layers when γ = 0.1

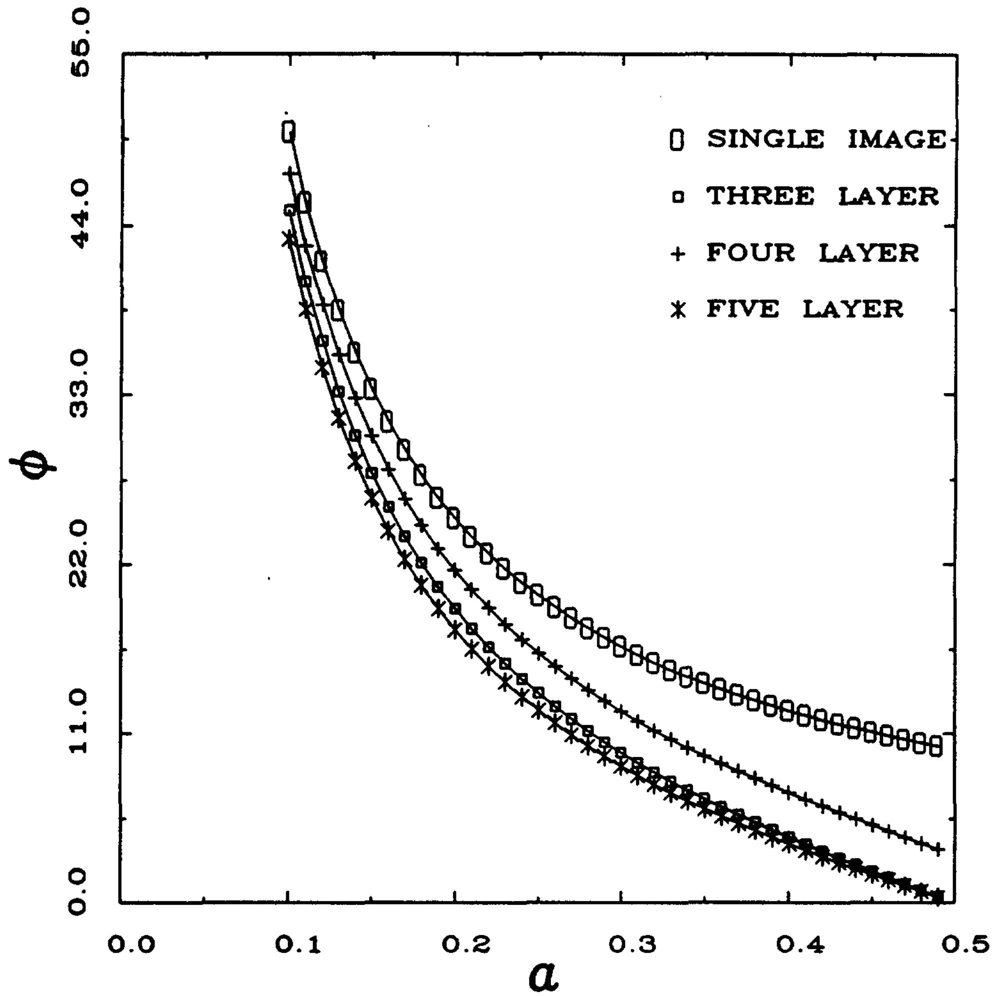

Fig. 4 Image force factor ϕ as a function of position a for three, four and five layers when $\gamma = 0.5$