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Evidence for screened-crystal-electric-field origin of the bulk and interfacial magnetoelastic stresses in Ho/Lu (0001) superlattices

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We present simple but quantitative theoretical evidence suggesting that the magnetoelastic (MEL) stress, which breaks the hexagonal symmetry of the basal plane in $(Ho_n/Lu_{15})\times 50$ (0001) superlattices ($n=8$–85 atomic planes, separated by $c/2$), has a single-ion crystal-electric-field (CEF) origin. The MEL stress M^γ has both a volume component M^γ_{vo} as well as an interface component M^γ_s. We show within the Hartree-Fock approximation that screening of the magnetostrictively distorted CEF by conduction-band electrons and the introduction of a spatial structure for the Ho^{3+} ionic charge are both needed to explain quantitatively the experimental values of $M^\gamma_{vo}=+0.275$ GPa and $M^\gamma_s/(c/2)=-7$ GPa; these effects are needed in particular to account for the different orders of magnitude and opposite signs. The simple point-charge model for bare ions in the magnetostrictively distorted CEF, as well as the simple free-electron screening approximation, both fail. [S0163-1829(98)50116-6]

Magnetoelastic (MEL) coupling in rare-earth (RE) superlattices is interesting because they are a good testing ground for simultaneously probing the bulk and interface (IF) MEL couplings. We previously determined[1] the MEL stress M^γ, which breaks the hexagonal basal-plane (bp) symmetry of the hcp structure in $(Ho_n/Lu_{15})\times 50$ (0001) superlattices, with $n_{Ho}=8$–85 atomic planes (ap's); we also studied such a symmetry breaking in Ho films of (5×10^3)-Å and 10^4-Å thicknesses. Details of the experimental procedure are given elsewhere,[2] as are details of the superlattices, which had good epitaxy of ~0.01–0.21 % and the interface roughness of only ± 2 ap (Refs. 2 and 3). We found that the strong experimental variation of M^γ with n_{Ho} could be rather well described, within the experimental uncertainty, by assuming that there were three contributions to M^γ, i.e.,[1]

$$M^\gamma = M^\gamma_{vo} + 2[M^\gamma_s/(c/2)]/n_{Ho} + \sigma_\epsilon . \tag{1}$$

The first term, M^γ_{vo}, is the unstrained lattice volume MEL stress; the second term is the interface MEL stress; and σ_ϵ is the average volume epitaxial stress, which arises because of the bulk bp lattice mismatch. From the fit we obtained, we determined M^γ_{vo} to be $+0.275$ GPa, (Ref. 4) and $M^\gamma_s/(c/2)$ to be -7 GPa, which results in a stress as large as $-6.4\, M^\gamma_{vo}$ for $n_{Ho}=8$. This large and negative value is remarkable and surprising, and needs to be explained. This is one of the aims of this work.

Since we are considering rare-earth superlattices, we assume for both the volume and interface components that the MEL coupling is of a single-ion character in a magnetostrictively distorted CEF. Therefore the MEL Hamiltonian for the basal plane (where Cartesian axes $\mathbf{x}\|\mathbf{a}$, $\mathbf{y}\|\mathbf{b}$; $\mathbf{a}$,$\mathbf{b}$ and $\mathbf{c}$ are the primitive vectors of the hcp unit cell) reads[5]

$$H_{me} = -\tilde{M}^{\gamma,2}\epsilon^\gamma_1 O^2_2(\mathbf{J}), \tag{2}$$

where $\epsilon^1_\gamma=(1/2)\ (\epsilon_{xx}-\epsilon_{yy})$, $\tilde{M}^{\gamma,2}$ is the *microscopic* MEL parameter, and $O^2_2(\mathbf{J})$ is the usual Stevens operator in terms of the Ho^{3+} $4f$-shell total angular momentum $\mathbf{J}$.

A model was earlier developed[6] to successfully calculate microscopic MEL parameters for cubic RE intermetallics, which we extend here to the RE hcp structure. Specifically, we expand the CEF potential produced by the surrounding ions and felt by the Ho^{3+} probe ion $V(\mathbf{r})$, and retain the term isomorphous of $O^2_2(\mathbf{J})$, i.e., $C^{\gamma,2}(x^2-y^2)$, with $C^{\gamma,2}=(1/2)(\partial^2 V/\partial x^2)_{r->0}$. We deform the lattice by the strain ϵ^1_γ and expand $C^{\gamma,2}$ around the unstrained lattice, thus obtaining

$$\tilde{M}^{\gamma,2} = -\alpha_J \langle r^2_{4f}\rangle (\partial C^{\gamma,2}/\partial \epsilon^1_\gamma)_{\epsilon^1_\gamma=0}, \tag{3}$$

where α_J is the reduced matrix element and $\langle r^2_{4f}\rangle$, the $4f$-electron average quadratic radius. We provide for a spatial structure to the ions surrounding the probe Ho^{3+}, in the form of a charge density with Gaussian shape of half-width d.[6] The potential produced by the ions is then screened by the conduction-band electrons. Working in the reciprocal lattice of the hexagonal one, of points $\mathbf{g}$, $V(\mathbf{r})$ is written as[7]

$$V(\mathbf{r}) = \sum_g \frac{v_p(\mathbf{g})}{\varepsilon(\mathbf{g})} \exp(-g^2 d^2) S(\mathbf{g}) \exp(i\mathbf{g}\cdot\mathbf{r}), \tag{4}$$

where $v_p(\mathbf{g})$ is the Fourier transform of the potential produced by an ionic point charge; $\varepsilon(\mathbf{g})$ is the Hartree-Fock (HF) or Linhard dielectric constant, taking into account electron-electron exchange within the Kohn-Sham approximation.[8] In this way we introduce positive Fermi holes, which, in principle, will reinforce the MEL parameter. $S(\mathbf{g})$ is the structure factor, for a unit cell ($\mathbf{a}$,$2\mathbf{b}$,$\mathbf{c}$), with four atomic sites (0,0,0), ($a/2$,b,0), ($a/2$,$b/3$,$c/2$), and (0,$4b/3$,$c/2$). When the crystal lattice $\mathbf{r}$ is deformed under ϵ^1_γ, preserving the volume, this deformation reverts to one of the reciprocal lattice $\mathbf{g}$.[6] Notice that $S(\mathbf{g})$ is invariant.[6] In this way we obtain $(\partial C^{\gamma,2}/\partial \epsilon^1_\gamma)_{\epsilon^1_\gamma=0}$ and finally, from Eq. (3),

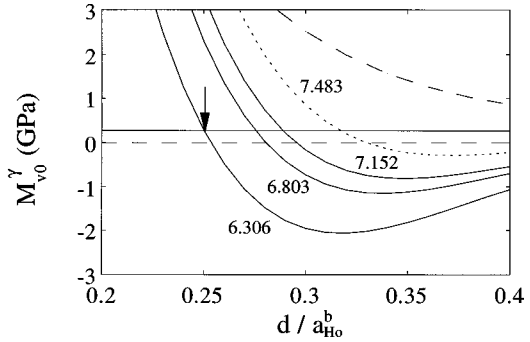

FIG. 1. The calculated volume magnetoelastic stress $M^{\gamma}_{\rm vo}$ against the ratio $d/a^{b}_{\rm Ho}$, where d is the radius of the Ho^{3+} ion and $a^{b}_{\rm Ho}$, the Ho basal plane lattice constant, for different situations: bare ions (discontinuous line); free-electron screening (dotted line); HF electron screening (full lines), with indication of the Fermi energies, $E^{\rm vol}_F$ (in eV). The DOE at the Fermi energy (in states/eV atom units) is 0.59 for free electrons and 1.78 for HF screening. The continuous horizontal line is the $M^{\gamma}_{\rm vo}$ value, at 0 K and saturation, as obtained from magnetoelastic stress measurements in the series of $(Ho_n/Lu_{15})\times 50$ (0001) superlattices ($n_{\rm Ho}=8-85$) (Ref. 1). $d/a^{b}_{\rm Ho}=0.25$ is the value for the bulk Ho metal. The vertical arrow signals the fitted $M^{\gamma}_{\rm vo}=+0.275$ GPa experimental value, for $E^{\rm vol}_F=6.306$ eV.

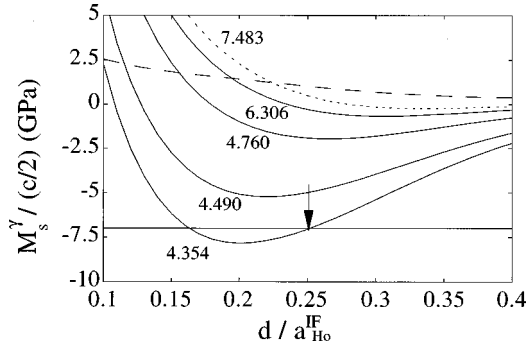

FIG. 2. The same as for Fig. 2 but for the calculated interface magnetoelastic stress divided by $c/2$, $M^{\gamma}_{s}/(c/2)$. The continuous horizontal line is $M^{\gamma}_{s}/(c/2)=-7$ GPa as obtained from the experiment (Ref. 1), in the way explained in the text. $a^{\rm IF}_{\rm Ho}$ is the basal plane lattice constant at the interface, at most 2% smaller than $a^{b}_{\rm Ho}$, and then we take $d/a^{\rm IF}_{\rm Ho}=0.25$ as for the bulk Ho. The vertical arrow signals the fitted $M^{\gamma}_{s}/(c/2)=-7$ GPa experimental value, for $E^{\rm IF}_F=4.354$ eV.

the MEL parameter $\tilde{M}^{\gamma,2}$. Its expression is given by Eqs. (A1) and (A2) of the Appendix. Our HF calculation assumes an average spherical Fermi surface (FS). However, a HF calculation of $\tilde{M}^{\gamma,2}$ using the Ho real electron band structure turns it into a formidable and analytically quite intractable problem.[6]

To compare with the experiment we need to relate the MEL parameter $\tilde{M}^{\gamma,2}$ with the MEL stress M^{γ}. The calculation is straightforward using the Callen & Callen standard theory of MEL coupling.[5] The result, for MEL stress at 0 K and at saturation (at an applied magnetic field of 12 T in the experiment[1]) is $M^{\gamma}=c_2 J^{(2)}\tilde{M}^{\gamma,2}$, a relation valid for the unstrained volume, $M^{\gamma}_{\rm vo}$ and interface M^{γ}_{s} MEL stresses. Notice that $c_2=2$ and $J^{(2)}=J(J-1/2)$.

We have calculated the parameter $\tilde{M}^{\gamma,2}_{v0}$ from Eqs. (A1) and (A2), summing up to $h+k+1=20$, where good convergence was obtained, choosing for d the Ho^{3+} ionic radius, 0.894 Å. For the unstrained lattice constant a_0 we take the bulk (^{b}) value $a^{b}_{\rm Ho}=3.578$ Å, because it differs from $a^{b}_{\rm SL}$ by less than 0.2%.[1–3] We then get $d/a_0\cong d/a^{b}_{\rm Ho}=0.25$. In Fig. 1 we plot the calculated volume stress $M^{\gamma}_{\rm vo}$ against $d/a^{b}_{\rm Ho}$, for the following different situations [densities of states (DOE's) are expressed in states/eV atom). For bare ions, and next for free electron screening for which in Ho, $E^{\rm vol}_F=7.48$ eV and $D(E^{\rm vol}_F)=0.599$. Both approximations clearly fail to reproduce the experimental value $M^{\gamma}_{\rm vo}=+0.275$ GPa (see Fig. 1). Band-structure calculations after the relativistic augmented plane-wave approximation[9] (RAPW) give, for Dy, $E^{\rm vol}_F=6.870$ eV and $D(E^{\rm vol}_F)=1.78$. If we adopt those values as starting ones for Ho, we are able to fit the experimental value of $M^{\gamma}_{\rm vo}$, at precisely $d/a^{b}_{\rm Ho}=0.25$, taking $E^{\rm vol}_F=6.306$ eV and $D(E^{\rm vol}_F)=1.78$ (see Fig. 1). We found that $M^{\gamma}_{\rm vo}$ was very insensitive to $D(E^{\rm vol}_F)$ variations, for the interval 0.599–1.78 the fitting value $E^{\rm vol}_F$ changing only by ≅6%. This is an indication that the use of a spherical FS is not as worse as it could be guessed. Notice, however, the rapid variation of $M^{\gamma}_{\rm vo}$ with $E^{\rm vol}_F$.

The calculation of the interface MEL stress $M^{\gamma}_{s}/(c/2)$ is more involved. We assume that the interface, on the Ho block side, is a single (0002) plane of Ho^{3+} ions symmetrically imbibed in a ''sheet'' of conduction electrons of width $c/2$.[10] The interface on the Lu side is of the same form, and both interfaces are sandwiched between Ho and Lu blocks. We will see later on that such an assumption works well. In such a scenario screening at the interface makes sense and conduction electrons can be treated as a three-dimensional system. Then to calculate $\tilde{M}^{\gamma,2}_{\rm IF}$ we simply set the **g** index $1=0$ in Eqs. (A1) and (A2). We have done the same kinds of calculations as for $M^{\gamma}_{\rm vo}$ and the results are shown in Fig. 2. We also take $b/a^{\rm IF}_{\rm Ho}=0.25$, because the epitaxial strain is at most $(a^{b}_{\rm Lu}-a^{b}_{\rm Ho})/a^{b}_{\rm Lu}=-0.018$, assuming perfect epitaxy.[1,3] We find that the value $M^{\gamma}_{s}/(c/2)=-7$ GPa is well reproduced taking a DOE $D(E^{\rm IF}_F)=1.78$ states/ eV atom, as in the bulk, but with a Fermi energy $E^{\rm IF}_F=4.35$ eV, *smaller* than the volume one. Notice that the Fermi wave vector and the Thomas-Fermi screening length were accordingly modified in Eqs. (A1) and (A2). Again the fitting $E^{\rm IF}_F$ value was very insensitive to $D(E^{\rm IF}_F)$, a variation of 0.05–1.78 produces a change of only −0.005 eV in $E^{\rm IF}_F$ (note that a DOE of ≈0.05 is about the expected one for a pure two-dimensional interface, with an average Ho block of $n_{\rm Ho}=35$ ap, although this is not our assumption).

We should stress that the Fermi *energies* or chemical potentials $E^{\rm vol}_F$ and $E^{\rm IF}_F$ are those determined before putting the Ho and Lu blocks in epitaxial contact, because of the calculation procedure followed for the MEL parameters. Indeed, after contact the conduction electrons will come to equilibrium with aligned Fermi *levels* for the Ho volume, the Ho^{3+} and Lu^{3+} interfaces, and the Lu volume. At the Ho^{3+} interface (the *only* one that can be probed magnetostrictively), this is achieved by an electron transfer from the Ho block to the Ho^{3+} interface, which gives rise to a dipolar layer with a potential difference, $\Delta V_{\rm Ho}=(E^{\rm vol}_F-E^{\rm IF}_F)_{\rm Ho}/e=1.94$ V, which

shifts together the electron levels and the chemical potential.[11,12] This shift is because of the modification of the charge density and periodic crystalline potential, within a distance $\cong c$ from the Ho/Lu ideal contact plane.[12] On the Lu side we should similarly get $\Delta V_{\mathrm{Lu}}=(E_F^{\mathrm{vol}}-E_F^{\mathrm{IF}})_{\mathrm{Lu}}/e$, and because the *epitaxial* contact potential between the Ho and Lu blocks must be $\Delta V_{\mathrm{Ho/Lu}}=[(E_F^{\mathrm{vol}})_{\mathrm{Ho}}-(E_F^{\mathrm{vol}})_{\mathrm{Lu}}]/e=6.306-6.16\cong 0.15$ V, then we should have $(E_F^{\mathrm{IF}})_{\mathrm{Ho}}=(E_F^{\mathrm{IF}})_{\mathrm{Lu}}$. Although the band electronic structures of bulk Ho and Lu are very close as well as the Fermi energies,[9] in principle, the Ho block band structure could be modified by interleaving Lu blocks, in turn modifying the volume MEL parameters to some extent. Therefore refinements in this direction of our simple model would be worth pursuing.

In order to gain insight into the difference found between the volume and interface Fermi energies, i.e., $E_F^{\mathrm{vol}}-E_F^{\mathrm{IF}}=1.95$ eV (we suppress the subscript ''Ho'' from hereafter), we have considered the hallmark simple Goodwin model[12,13] for the formation of quasifree electron states at the Ho^{3+} interface, for weak crystal potential. In spite of the crudity of this two-band model, their predictions remain basically valid when compared with more realistic recent models.[13] The model assumes that the Bloch function decays into the Ho block as $\exp(-qx)$, where x is the distance from the Ho/Lu ideal contact plane ($x=0$); therefore the Ho^{3+} interface electron states become weakly localized. Because the interface is around the (0002) plane, the hexagonal Brillouin zone (BZ) boundary at $\mathbf{K}/2=(\pi/c)\hat{\mathbf{c}}$ intersects both FS's, for the volume and the interface. Notice that now we are not assuming fully spherical FS surfaces. As is well known,[12,14] for such a boundary the gap is zero except for the line AH, where a gap is open because of the spin-orbit coupling, which at the point H amounts to $\Delta_{\mathbf{K}}\cong 0.46$ eV for Dy.[9] Although the gap is small it is essential for the formation of the interface states.[12,13] Then it can be easily shown, from the model calculated band structures at the interface and the bulk,[12,13] that the volume and interface Fermi energies differ as

$$E_F^{\mathrm{vol}}-E_F^{\mathrm{IF}}=(E_{F\|}^{\mathrm{vol}}-E_{F\|}^{\mathrm{IF}})+\frac{\hbar^2}{2m}q^2 \pm U_{\mathbf{K}}\left[1\mp\sqrt{1-\frac{E_0}{(U_{\mathbf{K}})^2}\,\frac{\hbar^2}{2m}q^2}\right], \qquad (5)$$

where $\Delta E_{F\|}\equiv E_{F\|}^{\mathrm{vol}}-E_{F\|}^{\mathrm{IF}}$ is the difference of electron kinetic energies parallel to the BZ hexagonal plane, with the Fermi wave vector $\mathbf{k}_F$ near to this plane and on the Fermi surface region close to the gap, both for the volume and the interface. $U_{\mathbf{K}}=\Delta_{\mathbf{K}}/2$ and $E_0=(\hbar^2/2m)(K/2)^2$. In Eq. (5) the upper (lower) sign refers to the upper (lower) band, along the BZ AH line. Notice the nearly s-electron character of those bands for bulk Ho,[9] which renders our spherical FS calculations more trustful.

Taking the determined difference $E_F^{\mathrm{vol}}-E_F^{\mathrm{IF}}=1.95$ eV, we have calculated from Eq. (5) q in terms of the difference $\Delta E_{F\|}$, assuming the FS lying in the two bands at point H of the BZ (Ref. 9) and therefore solving Eq. (5) for the upper band. We found the value $q=0.11$ Å^{-1}, corresponding to $\Delta E_{F\|}=1.68$ eV, for which the interface electron states decay in about $x=9.3$ Å, or at a distance $\cong 3(c/2)$ within the Ho block. This result agrees reasonably well with our above assumption of taking a Ho^{3+} interface of $c/2$ width, filled with conduction-band electrons, and with the above-followed procedure for calculating $\tilde{M}_{\mathrm{IF}}^{\gamma,2}$, i.e., setting the index $1=0$ in Eqs. (A1)–(A2). Therefore, it seems to us that the assumed simple Goodwin[12] model for electron band calculation at a RE metallic interface is reasonably satisfactory in explaining the found difference between the Fermi energies at the volume and the interface of our Ho_nLu_{15} superlattices, although as we said before some refining would be worthwhile in order to increase trust in the differences found in Fermi energies. Interfacial roughness effects of ± 2 ap could also play a role in producing the dipolar layer within the Ho block. Finally, notice that the effect of the epitaxial volume distortion at the interface is not important in producing such a Fermi-energies difference,[15] because if the interface electron concentration were kept constant and the epitaxial strain were assumed to be fully relaxed in the volume, for free electrons E_F^{IF} would *increase* only by $\cong 2\%$ with respect to E_F^{vol}, which is not the case.

To conclude we have shown that the gross features of MEL coupling in Ho/Lu (0001) superlattices can be explained by a quite simple model that considers a single-ion Ho^{3+} in the magnetostrictively distorted crystal electric field, combined with a Hartree-Fock approximation for the electron screening and endowing a spatial structure with the ionic charge density. The experimental values of the volume and interface MEL stresses can be both well reproduced if the Fermi energy, before epitaxy, of the interface is smaller than the volume one and if we take a density of states close to the obtained one from the bulk RAPW band-structure calculations for Dy. A simple although quantitative explanation has been given to the different Fermi-energy values, as a consequence of the assumed formation of Ho^{3+} interface weakly localized electron states close to the Ho/Lu ideal contact plane. However, two cautions are suggested. Small systematic variations with n_{Ho} of the volume contribution M_{vo}^{γ} (and of σ_{ϵ}) will result in variations of M_s^{γ}, although such an effect cannot be ascertained with our disposable experimental data. However, the sign and order of magnitude should probably be preserved, as both our volume and interface MEL parameters must be *single-ion* properties.[1,14,16] Therefore, a more refined theory of the conduction electron band structure for the whole superlattice could predict changes in the Ho volume MEL stress extended to a certain number of layers within the Ho block. We hope that our work can serve as a starting point for a better understanding and discussion of the MEL properties of rare earth superlattices.

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APPENDIX

The obtained expression for $M^{\gamma,2}$ is as follows:

$$\widetilde{M}^{\gamma,2}=\frac{\sqrt{6}\alpha_j\langle r_{4f}^2\rangle e^2}{a_0^3}\ \frac{4\pi Z_{\mathrm{RE}}}{9_{r_0}}\sum_{h,k,l}\exp[-\pi^2 d^2\hat{\mathbf{g}}^2/4a_0^2]$$
$$\times\frac{h^2}{\hat{\mathbf{g}}^2}\left[1+\frac{\hat{k}^2-\hat{l}^2}{\hat{\mathbf{g}}^2}\left(1+\frac{T}{2}\right)+\pi^2(\hat{k}^2-\hat{l}^2)\frac{d^2}{a_0^2}\right]S(\mathbf{g}) \tag{A1}$$

with

$$T\equiv-\frac{4\hat{k}_F^2+\hat{\mathbf{g}}^2}{4\hat{k}_F^2-\hat{\mathbf{g}}^2}+\left(\frac{\hat{\lambda}_0^2}{\hat{\mathbf{g}}^2}-\frac{\pi e^2 D(E_F)}{\hat{k}_F^2}\right)$$
$$\times\frac{1}{\varepsilon_0(\mathbf{g})}\ \frac{\hat{k}_F\sqrt{\hat{\mathbf{g}}^2}}{4\hat{k}_F^2-\hat{\mathbf{g}}^2}-2\frac{\hat{\lambda}_0^2\chi(\mathbf{g})}{\varepsilon_0(\mathbf{g})}, \tag{A2}$$

where: (h,k,l) are the components of the unstrained $\mathbf{g}$ vector with respect to the reciprocal lattice unit cell of the direct($\mathbf{a}$,2$\mathbf{b}$,$\mathbf{c}$) unit cell; $\hat{\mathbf{g}}^2=h^2+\hat{k}^2+\hat{l}^2$;$\varepsilon_0(\mathbf{g})$ is the well-known Hartree-Fock dielectric constant, with $\chi(\mathbf{g})$, the Lindhard response function;[8] $Z_{\mathrm{RE}}=+3$ for Ho^{3+}; $\hat{k}^2=k^2/3$; $r_0=c_0/a_0$; $\hat{l}^2=1^2/{r_0}^2$; $\hat{k}_F=k_F/(2\pi/a_0)$, with $\mathbf{k}_F$ being the Fermi wave vector, assuming an effective spherical Fermi surface, i.e., $E_F=(\hbar^2/2m)k_F^2$, with E_F being the Fermi energy; and $\hat{\lambda}_0^2=\lambda_0^2/(2\pi/a_0)^2$, with $\lambda_0=[4\pi e^2 D(E_F)]^{1/2}$, the inverse of the screening Thomas-Fermi length. The subscript ''0'' means values for the magnetostrictively unstrained lattice. Notice that in Eq. (A2) the term $-[\pi e^2 D(E_F)/\hat{k}_F^2)$ stands for the conduction-band electron exchange of Kohn-Sham type.[8] Equations (A1) and (A2) both apply to the volume and the interface with the appropriate election of the magnitudes involved, as explained in the text.

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