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SPATIAL MOMENTS OF PHASE DENSITY OF A FLUX OF CASCADE ATOMS IN KINETIC THEORY OF SPUTTERING FERROMAGNETICS

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The kinetic equations describing ion interactions with a ferromagnetic target have been found and solved. The main spatial (Z-coordinate at a normal to the target surface under bombardment) moments of the density distribution of atoms moving in a cascade have been found. The moments found are used to restore the form of the function determining the target sputtering yield for the Gaussian approximation in a broad temperature range including the region of magnetic phase transition.

Key Words : Spatial Moments; Phase Density; Flux; Cascade Atoms; Kinetic Theory; Sputtering Ferromagnetics; Gaussian Approximation

IN this work, consideration is being given to a concrete system, viz., an ion beam interaction with a ferromagnetic target. Then, by analogy of Sigmund's sputtering theory,[1] the following balance equations may be written for phase densities of a flux of cascade atoms whose spins are directed "upwards", $\phi^{(1)}$, and "downwards" $\phi^{(2)}$:—

$$\frac{1}{v}\frac{\partial}{\partial t}\phi^{(1)}(\mathbf{r},\boldsymbol{\varphi},E,t) + \boldsymbol{\varphi}\nabla_r\phi^{(1)}$$

$$= -\pi a^2 n_1\phi^{(1)} - \pi A^2 n_2\phi^{(1)}$$

$$+ n_1 \int\limits_{1\geqslant \boldsymbol{\varphi}\boldsymbol{\varphi}' > \sqrt{\frac{E}{E_0}}} \mathrm{d}\varphi \int_E^{E_0} \mathrm{d}E'\sigma_a(\boldsymbol{\varphi}', \to \boldsymbol{\varphi}; E' \to E)\,\phi^{(1)}(\mathbf{r},\boldsymbol{\varphi}'E',t)$$

$$+ n_1 \int\limits_{1\geqslant \boldsymbol{\varphi}\boldsymbol{\varphi}' > \sqrt{\frac{E}{E_0}}} \mathrm{d}\boldsymbol{\varphi}' \int_E^{E_0} \mathrm{d}E'\sigma_a(\boldsymbol{\varphi}' \to \boldsymbol{\omega}; E' \to E' - E)\,\phi^{(1)}(\mathbf{r},\boldsymbol{\varphi}',E',t)$$

$$+ n_2 \int\limits_{1\geqslant \boldsymbol{\varphi}\boldsymbol{\varphi}' > \sqrt{\frac{E}{E_0}}} \mathrm{d}\boldsymbol{\varphi}' \int_E^{E_0} \mathrm{d}E'\sigma_A(\boldsymbol{\varphi}' \to \boldsymbol{\varphi}; E' \to E)\,\phi^{(1)}(\mathbf{r},\boldsymbol{\varphi}',E',t)$$

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$$+ n_1 \int\limits_{1 \geqslant \varphi\varphi' > \sqrt{\frac{E}{E_0}}} d\varphi' \int\limits_{E}^{E_0} dE' \sigma_A(\varphi' \rightarrow \omega; E' - E' - E)\, \phi^{(2)} (\mathbf{r},\varphi',E',t). \quad ...(1)$$

The equation for $\phi^{(2)}$ is completely analogous to eq. (1), except the substitution (1) $\leftrightarrows$ (2).

The initial and final conditions are

$$\phi^{(1)}(\mathbf{r}, \varphi, E, 0) = \nu\delta(\mathbf{r})\,\delta(\varphi - \varphi_0)\,\delta(E - E_0)$$

$$\left\{\delta(\varphi - \varphi_0) = \frac{1}{2\pi}\,\delta(\cos\vartheta - 1)\right\}$$

and

$$\phi^{(1)}(t \rightarrow \infty) = \phi^{(2)}(t \rightarrow \infty) = \phi^{(2)}(t = 0) = 0,$$

respectively. Obviously, we seek for the total number S of the particles (the total flux) which penetrate the plane Z = const within the time of particle residence in the cascade and whose velocity component along the Z-axis is either positive (S^+) or negative (S^-). For the spin-insensitive detectors, the equations for S^+ and S^- are

$$S^+(Z) = \int\limits_0^\infty dt \int\limits_{-\infty}^{+\infty}\int dx dy \int\limits_E^{E_0} dE \int\limits_{\varphi n^+ \geqslant 0} d\varphi(\varphi n^+)\,(\phi^{(1)}(\mathbf{r}\varphi,E,t) + \phi^{(2)}(\mathbf{r},\varphi,E,t)\; \varphi\mathbf{n}^+ = \{0,0,1\}. \quad ...(2)$$

$$S^-(Z) = \int\limits_0^\infty dt \int\limits_{-\infty}^{+\infty}\int dx dy \int\limits_E^{E_0} dE \int\limits_{\varphi \mathbf{n}^- > 0} d\varphi(\varphi\mathbf{n}^-)\,(\phi^{(1)}(\mathbf{r},\varphi,E,t) + \phi^{(2)}(\mathbf{r},\varphi,E,t)\; \{\mathbf{n}^- = 0,0,-1\}. \quad ...(3)$$

These equations are written for normal ion incidence. The case of oblique incidence was treated by Sigmund.[2] It should be noted that S^- corresponds to so called "backward sputtering yield," while S^+ corresponds to the "transmission sputtering."

Now we shall assume that $\pi a^2 n = \sigma$ and expand the functions in (1), (2) and (3)in the Legendre polynomials :

$$\phi(Z,\eta',E') = \frac{1}{4\pi}\sum_{k=0}^{\infty}(2k+1)\,P_k(\eta')\,\phi_k(E,E'); \quad ...(4)$$

$$\Theta\left(\mu - \sqrt{\frac{E}{E_0}}\right)\delta\left(\mu - \sqrt{\frac{E}{E'}}\right) = \frac{1}{4\pi}\sum_{k=0}^{\infty}(2k+1)\Lambda_k\,P_k(\mu);\; (\mu = \varphi\varphi') \quad ...(5)$$

Substituting (4), (5) in (2), (3) and integrating over time and X, Y, we get

$$S^{+}(Z) = 2\pi \int_{-1}^{+1} \eta\Theta(\eta)\, d\eta \left\{ \frac{1}{4\pi} \sum_{k=0}^{\infty} (2k+1)\, P_k(\eta) \int_{u(\eta)}^{E_0} \left(\phi_k^{(1)} + \phi_k^{(2)} \right) dE \right\} \quad ...(6)$$

and $$S^{-}(Z) = -\, 2\pi \int_{-1}^{+1} \eta\Theta(\eta)\, d\eta \left\{ \frac{1}{4\pi} \sum_{k=0}^{\infty} (2k+1)\, P_k(\eta) \int_{u(\eta)}^{E_0} \left(\phi_k^{(1)} + \phi_k^{(2)} \right) dE \right\} \quad ...(7)$$

Here $\phi_k^{(1)}$ and $\phi_k^{(2)}$ are the coefficients of the Legendre polynomials in the expansion of the integrated over t, x, y phase densities of the flux of cascade atoms with spins "upwards" and "downwards" respectively. After introducing the designations

$$\pi\, a^2 n_1 = \sigma_1,\ \pi a^2 n_2 = \sigma_2;\ \pi A^2 n_1 = \Sigma_1;\ \pi A^2 n_2 = \Sigma_2,$$

we set

$$\phi_k^{(1)}(Z, E) = \delta(E - E_0)\, \Theta(Z) \exp\{ -(\sigma_1 + \Sigma_2) Z \} + \tilde{\phi}_k^{(1)}(Z, E), \quad ...(8)$$

where $\phi_k^{(1)}(Z, E)$ is regular function near E_0, $Z = 0$. By this, we have singled out the contribution of the particles which acquired an initial momentum.

The spatial moments of the function $\phi(Z, E)$ are determined by the formula

$$\phi_m(E) = \int_{-\infty}^{+\infty} Z^m \phi(Z, E)\, dZ, \quad ...(9)$$

whence the equations for the spatial moments are

$$(\sigma_1 + \sigma_2)\, \tilde{\phi}_{k;m}^{(1)}(E) = m \left[\frac{k+1}{2k+1} \tilde{\phi}_{k+1;m-1}^{(1)}(E) + \frac{k}{2k+1} \tilde{\phi}_{k-1;m-1}^{(1)}(E) \right]$$
$$+ (2\sigma_1 + \Sigma_2) \int_{E}^{E_0} \frac{dE'}{E'} P_k\left(\sqrt{\frac{E}{E'}} \right) \tilde{\phi}_{k;m}^{(1)}(E')$$
$$+ \Sigma_1 \int_{E}^{E_0} \frac{dE'}{E'} P_k\left(\sqrt{\frac{E}{E}} \right) \phi_{k;m}^{(2)}(E')$$
$$+ \frac{m!}{E_0} P_k\left(\sqrt{\frac{E}{E_0}} \right) \frac{2\sigma_1 + \Sigma_2}{(\sigma_1 + \Sigma_2)^{m+1}}; \quad ...(10)$$

$$(\sigma_2 + \sigma_1)\, \phi_{k;m}^{(2)}(E) = m \left[\frac{k+1}{2k+1} \phi_{k+1;m-1}^{(2)}(E) + \frac{k}{2k+1} \phi_{k+1;m-1}^{(2)}(E) \right.$$

(eqn. contd.)

$$+ (2\sigma_2 + \Sigma_1 \int_E^{E_0} \frac{dE'}{E'} P_k\left(\sqrt{\frac{E}{E'}}\right) \phi^{(2)}_{k;m}(E')$$

$$+ \Sigma_2 \int_E^{E_0} \frac{dE'}{E'} P_k\left(\sqrt{\frac{E}{E'}}\right) \tilde{\phi}^{(1)}_{k;m}(E')$$

$$+ \frac{m!}{E_0} P_k \left(\sqrt{\frac{E}{E_0}}\right) \frac{\Sigma_2}{(\sigma_1 + \Sigma_2)^{m-1}} \quad \text{...(11)}$$

To find $\phi^{(1)}_{k;m}(E)$; $\phi^{(2)}_{k;m}(E)$, we shall reduce the integral equations by differentiation to the Euler equations[3] which will be solved further by the method of varying constant. This method was used to find the following moments as functions of energy :

$$\phi_{0;0}(E) = \frac{2E_0(\Sigma_1 + \Sigma_2)}{[\Sigma_1(\sigma_1 + \Sigma_2) + \Sigma_2(\sigma_2 + \Sigma_1)]} \frac{1}{E^2}$$

$$+ \frac{\alpha E_0^{\alpha-1} \Sigma_2 [(\sigma_2 + \Sigma_1) - (\sigma_1 + \Sigma_2)]}{[\Sigma_1(\sigma_1 + \Sigma_2) + \Sigma_2(\sigma_2 + \Sigma_1)] (\sigma_1 + \Sigma_2)} \frac{1}{E^\alpha} = \frac{C}{E^2} + \frac{D}{E^\alpha};$$

$$\phi_{0;1}(E) = \frac{10 E_0}{(\sigma_1 + \Sigma_2)(\sigma_2 + \Sigma_1)} \frac{1}{E^2} - \frac{E_0}{(\sigma_1 + \Sigma_2)(\sigma_2 + \Sigma_1)} \frac{1}{E^{3/2}} \quad \text{...(13)}$$

$$\phi_{1;1} = \tfrac{5}{3}\, \phi_{0;0}(E) \frac{\Sigma_1(\sigma_2 + 2\Sigma_2 + 3\Sigma_1) + \Sigma_2(\sigma_1 + 2\Sigma_1 + 3\Sigma_2)}{(\Sigma_1 + \Sigma_2)[(\sigma_1 + 3\Sigma_2)(\sigma_2 + 3\Sigma_1) - 4\Sigma_1\Sigma_2]}; \quad \text{...(14)}$$

$$\phi_{0;2} = \phi_{0;0}\, \phi_{1;1} \quad \text{...(15)}$$

$$\phi_{1;2} = 5 \frac{(\sigma_2 + 3\Sigma_1 + 2\Sigma_2)\left(2\phi^{(1)}_{2,2} + \phi^{(1)}_{0,2}\right)] + \left[(\sigma_1 + 3\Sigma_2 + 2\Sigma_1) \times \left(2\phi^{(2)}_{2,2} + \phi^{(2)}_{0,2}\right)\right.}{(\sigma_1 + 3\Sigma_2)(\sigma_2 + 3\Sigma_1) - 4\Sigma_1\Sigma_2} \quad \text{...(16)}$$

$$\phi_{2;2} = \frac{16}{5} \frac{(2\sigma_2 + 3\Sigma_1 + \Sigma_2)\tilde{\phi}^{(1)}_{1,1} + (2\sigma_1 + 3\Sigma_2 + \Sigma_1)\phi^{(2)}_{1,1}}{(2\sigma_1 + 3\Sigma_2)(2\sigma_2 + 3\Sigma_1) - \Sigma_1\Sigma_2} \quad \text{...(17)}$$

The found spatial moments $\phi_{k;m}$ are used to determine the moments $S^+_{k;m}$, $S^-_{k;m}$ which are used, in turn, to restore the yields of transmission sputtering and of backward one. The main purpose of this paper is a methodical one. The problem in interest was to detect the dependence of spatial momenta on spin orientation in very simple model of ferromagnet with two spin states only. However, the direct comparison with the relevant experimental findings is possible for Ni sputtering. As it is known, the spin properties of Ni are close to properties of our model with limiting condition $S = 1/2$. For this reason the detailed theoretical treatment on backward sputtering yield of Ni was performed according to this model recently.[5] The difference between yields in ferromagnetic state and paramagnetic one was found to be about 10–12 per cent. This calculated data are in a good agreement with availabl experimental results.[5,6] It should be noted that change spatial distribution of moving atoms in cascade contribute to yield variation under magnetic phase transition. The remainder contribution is due to variation of surface bidding energy under phase transition.

The more realistic model for sputtering of ferromagnets with arbitrary spins was considered by Motaweh *et al.* (*to be published*) and by Karpova.[7] In these works the authors studied the sputtering yield of lanthanaides-4f-shell rare-earth magnets with indirect exchange interaction. There was the theoretical prediction not only relative but absolute value of sputtering yield for Gd, Tb, Dy under magnetic phase transition for Ne, Ar, Kr, Xe bombarding ions. There is good agreement with available experimental data.[8]

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