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AN EVALUATION OF LONG-WAVELENGTH SURFACE PLASMON DISPERSION COEFFICIENT 'α' FOR VARIOUS SIMPLE METAL SURFACES

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ABSTRACT

This paper presents an evaluation of long wavelength surface plasmon dispersion coefficients α (Å) for various simple metal surfaces using various models (HD, SRM, IBM, RPA and ALDA). It was observed that the surface plasmon dispersion coefficient 'α' evaluated using RPA and ALDA models are negative as per experimental observation but the magnitude is large. On the other hand, 'α' calculated from HD and SRM models are positive but the magnitude matches with experimental data.

Key words: Surface plasmon dispersion coefficient, Hydrodynamics models, Specular reflection models. Random phase approximation, Nonlocal effects.

INTRODUCTION

In the pioneering treatement of characteristics energy loses of fast electrons passing through thin metal films, Ritchie[1] predicted the existence of self sustained collective excitations at metal surface. Pines and Bhom[2, 3] had already pointed that the long range nature of the coulombs interaction between valance electrons in metals yields collective plasmon oscillations similar to the electron density oscillations observed by Tonks and Langmuir in electrical discharge in gases[4]. Ritchie[1] showed that the boundary effect is the cause of appearance of new lowered loss due to the excitation of surface collective oscillations. Powell and Swan[5] demonstrated through electron energy loss experiment, the existence of these collective excitations. Stern and Firrel[6] called the quanta of these collective excitations as surface plasmon.

Since then, there has been significant advancement in both theoretical and experimental investigations of surface plasmon. These studies have played a key role in the

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field of condensed matter and surface physics. Now a days, a field has emerged called plasmonics, which represents an exciting area for the application of surface plasmons. In this field, surface plasmon based circuits are used in the field of photonics and electronics at the nanoscale[7].

According to the work of Pines and Bhom, the quantum energy oscillations in a free electron gas with equilibrium density n is $\hbar\omega_p = \hbar(4\pi ne^2/m_e)^{1/2}$, ω_p being the so-called plasmon frequency. In the case of planer boundary, there is a new mode (the surface plasmon) the frequency of which equals to Richie frequency $\omega_s = \omega_p/\sqrt{2}$ in the non-retarded region (where the speed of light can be taken to be infinity large). This frequency exists at wave-vector q in the range $\omega_s << q << q_F$ (q_F being the magnitude of Fermi wave vector). It also exhibits some dispersion as the wave vector is increased. In the retarded region, where the phase vector ω_s/q of the surface plasmon is compared to the velocity of light, surface plasmons couple with the free electromagnetic field. These surface plasmon propagate along the metal surface with frequency ranges from zero at (q = 0) towards the asymptotic value $\omega_s = \omega_p/\sqrt{2}$.

In the case of thin films, the electric fields of both surfaces interact. As a result, there are (i) tangential oscillation characterized by a symmetric disposition of charge deficiency or excess of opposing points on the two surface (ii) normal oscillations in which an excess of charge density at a point on one surface is accompanied by a deficiency at the point directly across the thin film. The phase velocity of the tangential surface plasmon is always larger than the speed of light as it occurs in the case of a semi-infinite electron system. The phase velocity of normal oscillations may surpass that of light; thereby becoming a radiative surface plasmons that is responsible for the emission of light[8]. This radiation was detected[9,10] using electron beam bombardment of thin film of Ag, Mg, and Al with thickness ranges between 5 to 1000Å. Light emission was observed[11] in the ultraviolet from a metal-oxide metal tunnel diode and was attributed to the excitation of the radiation surface plasmon.

In this paper, surface plasmon dispersion coefficient α (Å) have been evaluated for various simple metals using various theoretical models proposed[12-16] in this study. We have compared our theoretical results with the experimental data[17,18] obtained through angle resolved low energy inelastic electron scattering, which shows that the surface plasmon energy of simple metal dispersion downward in energy at small momentum q parallel to the surface.

Mathematical formulae used in the evaluation

The simplest models for surface plasmon is jellium surface in vacuum. Here, a semi-infinite medium with local dielectric function $\epsilon(\omega)$ at $z \leq 0$ is determind at $z = 0$. The surface response function $g(q,\omega)$ is obtained[19] -

$$g(q,\omega) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1} \quad \ldots(1)$$

Keeping $\epsilon_2 = 1$

Now for derived dielectric function[20], one has surface loss function -

$$I_m\, g(q, \omega) = (\pi / 2)\, \omega_s\, \delta(\omega - \omega_s) \quad \ldots(2)$$

Where $\omega_s = \omega_p/\sqrt{2}$

The classical energy loss function of equation (1) represents the long wavelength ($q \rightarrow 0$) limit of the actual self consistent surface loss function of Jillium surface. The classical picture given by equation (1) ignores both; the non-locality of the electronic response of the system and the microscopic spatial distribution of the electron near the surface. Non-locality effect can be incorporated within the hydrodynamic model[12] (HD) and specular reflection model[13] (SRM). One has dispersion of the surface plasmon using quantum hydrodynamic approach.

$$\omega^2 = \tfrac{1}{2} [\omega_p^2 + \beta^2 q^2 + \beta q(2\omega_p^2 + w^2 q^2)^{1/2}] \quad \ldots(3)$$

at long wavelength yields

$$\omega = \omega_p/\sqrt{2} \quad + \beta q/2 \quad \ldots(4)$$

β represents the speed of propagation of hydrodynamic distribution within the electron system ($\beta q/\omega_p << 1$ but $\omega/c << q$).

In the SRM (with the bulk dielectric function being described within RPA) surface plasmon are damped by the presence of p-h existence. Now hydrodynamic equation (3) and (4) and a numerical evaluation of the imaginary part of the SRM surface response function both yield positive surface plasmon energy dispersion at all wave vectors. But Benett[21] used a hydrodynamic model with a continuum decrease of the electron density at the metal surface and found that a continuous electron density variation yields a monopole surface plasmon with negative dispersion at low wave function.

Self – consistence calculations

Within the self consistent long wavelength dispersion of the Jillium-surface electronic response, Kibelman[22] showed that up to first order in an expension in power of the magnitude q of the wave under the surface response function can be written as -

$$g(q,\omega) = \frac{[\in(\omega) - 1]\,[1 + qd_{\perp}(\omega)]}{[\in(\omega) + 1 - [\in(\omega) - 1]\,qd_{\perp}(\omega)} \quad \ldots(5)$$

Where $\in(\omega)$ is the long wavelength limit of the dielectric function of the bulk material and $d_{\perp}(\omega)$ is the centroid of the induced electron density with respect to the Jellium edge. From equation (5), one gets surface plasmon dispersion relation for semi-infinite electron metal in vacuum.

$$\omega = \omega_s (1 + \alpha q) \quad \ldots(6)$$

where,

$$\alpha = -\mathrm{Re}\,[d_{\perp}(\omega_s)]/\sqrt{2} \quad \ldots(7)$$

These relation shows a negative dispersion coefficients.[20,21]

Quantitative RPA calculation were carried out by several authors[23-25] by using specular reflection and infinitive-barrier models (IBM)[26], step potential[27] and more relativistic Long-Kohn self consistent surface potential[27]. Both Feibelman's RPA self consistent calculations[28] and the ALDA calculation carried out by Liebsel[16] and Kempa and Schaich[28] showed that in the range of typical bulk densities (r_s = 2~6), the centroid of the induced electron density at - ω_s lies outside the Jellium edge, which leads to a negative long wavelength dispersion of the surface plasmon. Now hydrodynamic coefficient α^{HD} obtained from hydrodynamic models is given by[12] -

$$\alpha^{HD} = \beta / 2\omega_s \quad \ldots(8)$$

This model shows that in the long wavelength plasmon, dispersion is always positive.

RESULTS AND DISCUSSION

We have evaluated the long wavelength ($q \rightarrow 0$) surface plasmon dispersion coefficient 'α' for various simple metals. The results are shown in Table 2. We have also evaluated α (Å) as a function of electron density parameters 'r_s' for various theoretical

models namely HD, SRM, IBM, RPA and ALDA. We have taken equation (6) and (7) in these evaluations. We have taken this surface plasmon frequency as -

$$\omega s = \omega p/\sqrt{2} = \left(\frac{3}{2r_s^3}\right)^{1/2} \frac{e^2}{\alpha_0} \quad \ldots(9)$$

We have compared our theoretical results with the experimental data of the surface plasmon dispersion coefficient measured from angle resolved long energy inelastic electron scattering. From our calculation, it shows that self-consistent RPA and ALDA calculation are in reasonable agreement with the experimental data. It also indicates that the surface plasmon energy of simple metal dispersion downward in energy at small momentum q parallel to the surface. The volume plasmon energy has quadrative dependence on the momentum transfer q with positive plasmon dispersion coefficients[29-32]. The surface plasmon and surface plasmon polarization were recently studied by several workers[33-36].

Table 1: An evaluated result of surface plasmon dispersion coefficient α (Å) as a function of electron density r_s using various models

r_s	α (Å)			
	RPA	**ALDA**	**IBM**	**SRM**
0.5	- 0.15	- 0.22	-	0.25
1.0	- 0.16	- 0.25	-	0.32
1.5	- 0.20	- 0.29	0.24	0.32
2.0	- 0.22	- 0.33	0.30	0.39
2.5	- 0.28	- 0.45	0.37	0.47
3.0	- 0.32	- 0.68	0.33	0.58
3.5	- 0.38	- 0.75	0.32	0.65
4.0	- 0.47	- 0.84	0.30	0.68
4.5	- 0.42	- 0.96	0.30	0.74
5.0	- 0.38	- 1.15	0.30	0.80
5.5	- 0.32	- 1.18	0.30	0.84
6.0	- 0.27	- 1.22	0.30	0.86

Table 2: An evaluated results of surface plasmon dispersion coefficient α in Å for various simple metal surfaces obtained from various theoretical models. The results are compared with experimental data.

Metal surfaces	r_s	ω_s	α (Å)					
			HD	**SRM**	**IBM**	**RPA**	ALDA	Expt
Al	2.07	10.86	0.46	0.41	0.38	- 0.24	- 0.34	- 0.32
Mg	2.66	7.38	0.52	0.49	-	- 0.30	- 0.56	- 0.47
Li	3.25	4.28	0.58	0.62	0.35	- 0.33	- 0.71	- 0.24
Na	3.93	3.99	0.64	0.66	-	- 0.44	- 0.82	- 0.39
K	4.86	2.74	0.71	0.72	-	- 0.39	- 1.11	- 0.31
Cs	5.62	1.99	0.76	0.85	0.35	- 0.29	- 1.20	- 0.44

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