



# Kramers–Kronig transform for the surface energy loss function

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## Abstract

A new pair of Kramers–Kronig (KK) dispersion relationships for the transformation of surface energy loss function  $\text{Im}[-1/(\varepsilon + 1)]$  has been proposed. The validity of the new surface KK transform is confirmed, using both a Lorentz oscillator model and the surface energy loss functions determined from the experimental complex dielectric function of SrTiO<sub>3</sub> and tungsten metal. The interband transition strength spectra ( $J_{cv}$ ) have been derived either directly from the original complex dielectric function or from the derived dielectric function obtained from the KK transform of the surface energy loss function. The original  $J_{cv}$  trace and post- $J_{cv}$  trace overlapped together for the three modes, indicating that the new surface Kramers–Kronig dispersion relationship is valid for the surface energy loss function.

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## 1. Introduction and literature survey

Quantitative optical properties are playing an increasingly important role in electronic structure studies of materials [1]. All optical properties can be derived from the complex dielectric function  $\varepsilon(\omega)$ . This function is therefore of prime importance, and can be determined in many ways, using either incident photons or electrons. In the VUV range (up to  $E = 100$  eV, where  $E = \hbar\omega$ ), optical reflectance measurements probe bulk materials and require well-polished samples [2–4]. The use of transmission electron energy loss spectroscopy (TEELS) probes the bulk energy loss function  $\text{Im}[-1/\varepsilon(\omega)]$  [5]. The spatial resolution in TEELS in the electron microscope allows probing the very local dielectric properties of nanometer thick interfacial films, [6] or grain boundaries [7]. However, TEELS requires specially prepared samples, in the form of thin, electron transparent foils.

All these methods require a Kramers–Kronig transformation of the experimentally acquired data, which allows determination of one conjugate part of a complex optical property once the other part has been experimentally obtained. For example in SrTiO<sub>3</sub> such an approach has shown that the  $\varepsilon(\omega)$  functions derived from Kramers–Kronig analysis of optical reflectance from VUV measurements and of the bulk energy loss function from TEELS measurements were comparable [8]. In addition,  $\varepsilon(\omega)$  profiles across grain boundaries could be obtained from TEELS [9] demonstrating the interfacial electronic structure of grain boundaries in SrTiO<sub>3</sub>.

Kramers–Kronig analysis of electron energy loss function measurements in the transmission mode (TEELS) using high-energy electrons is a well-established method [5,10–12] to determine the optical properties of a solid over a wide energy range. Within the range of validity of the dielectric theory, the probability that an electron traveling in a medium of dielectric function  $\varepsilon(\mathbf{q}, E)$ , suffering an inelastic scattering process characterized by a momentum transfer  $\mathbf{q}$  and an energy loss  $E$ , is determined by the energy loss function (ELF)  $\text{Im}[-1/\varepsilon(\mathbf{q}, E)]$ . Within the optical limit ( $\mathbf{q} \rightarrow 0$ ) both the transverse and lon-

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itudinal dielectric constant ( $\varepsilon(0,E)$ ) coincide [13] so that the TEELS spectra will approach the optical energy loss function  $\text{Im}[-1/\varepsilon(0,E)]$ . Thus the Kramers–Kronig analysis enables the determination of optical properties. In the following, we denote the energy loss either by  $E$  or by  $\hbar\omega$ .

As the dielectric response function is causal, a Kramers–Kronig transformation [11] can be used to derive the function  $\text{Re}[1/\varepsilon(\omega)]$  from  $\text{Im}[-1/\varepsilon(\omega)]$ :

$$\text{Re} \left[ \frac{1}{\varepsilon(\omega)} \right] - 1 = -\frac{2}{\pi} P \int_0^\infty \text{Im} \left[ \frac{-1}{\varepsilon(\omega')} \right] \frac{\omega' d\omega'}{\omega'^2 - \omega^2} \quad (1)$$

$$\text{Im} \left[ \frac{-1}{\varepsilon(\omega)} \right] = \frac{2}{\pi} P \int_0^\infty \frac{\text{Re}[1/\varepsilon(\omega')] - 1}{\omega'^2 - \omega^2} d\omega' \quad (2)$$

Here  $P$  denotes the Cauchy principal part of the integral, avoiding the pole at  $\omega = \omega'$ . In Eqs. (1) and (2), the factor  $\omega'/(\omega'^2 - \omega^2)$  acts as a “weighting function”, giving prominence to energy losses  $\hbar\omega'$ , which lies close to  $\hbar\omega$ .

$\text{Im}[-1/\varepsilon]$  is given an absolute scale by use of a Kramers–Kronig sum rule [11] the index sum rule, obtained by setting  $\omega = 0$  in Eq. (1):

$$1 - \text{Re} \left[ \frac{1}{\varepsilon(0)} \right] = \frac{2}{\pi} \int \text{Im} \left[ \frac{-1}{\varepsilon(\omega)} \right] \frac{d\omega}{\omega} \\ = \frac{2}{\pi} \int [\text{Scale\_factor} \times \text{data}] \frac{d\omega}{\omega}. \quad (3)$$

Since  $\text{Re}[1/\varepsilon(0)] = \varepsilon_1/(\varepsilon_1^2 + \varepsilon_2^2)$ , the left hand side of Eq. (3) can be taken as unity for a metal, where both  $\varepsilon_1$  and  $\varepsilon_2$  become very large at  $\omega \rightarrow 0$ . In case of an insulator,  $\varepsilon_2$  is small for small  $\omega$  and  $\text{Re}[1/\varepsilon(0)] \cong 1/\varepsilon_1(0)$ , where  $\varepsilon_1(0)$  is the square of the refractive index for visible light.

Materials for advanced applications in electronics are very often in the form of surficial films with nanometer thickness. Therefore, VUV optical measurements are not always well-suited, as the substrate is also probed, due to the large optical probing depth in the VUV (which can be greater than 100 nm), and TEELS also probes the depth of the sample, and can only detect the bulk energy loss function.

For such materials, when the surficial film is of primary interest, one can use low energy electrons (from 20 eV to 1000 eV), and take the electron energy loss spectra in the reflection mode (REELS, reflection electron energy loss spectroscopy). Due to the small inelastic mean free path (IMFP) of electrons, which determines the probing depth, only the surficial film will be probed if the electron energy is low enough that the IMPF is smaller than the thickness of the thin films. Therefore, the surficial electronic structure and physical properties of the surficial films, such as complex dielectric function as well as optical constants, could be determined from REELS if the surface and bulk energy loss function could be successfully separated each other from REELS spectrum.

Since the probing depth in REELS is very small (around several nanometers), the excitation from the surficial films by the incident electrons is much more complicated than that in TEELS. Both bulk and surface excitations contribute to

REELS [13,14]. The relative contribution of each depends on the primary energy and may be expressed as a mathematical formula [15]. Many attempts have been made in the literature to derive from the REELS spectrum the complex dielectric function  $\varepsilon(\omega)$ ; most of them treat REELS as a mixture of surface and bulk excitation. Some considered the REELS spectrum to be a linear combination of bulk and surface energy loss function (ELF) [16,17]. The dielectric function was then either obtained by an iterative procedure, beginning with the assumption that the REELS spectrum reflects the bulk ELF, or by choosing a test function  $\text{Im}[-1/\varepsilon(\omega)]$  [17]. In all these approaches, the surface and bulk contributions are derived from the bulk dielectric function, assuming implicitly that the dielectric function at the surface is the same as in the bulk, which might not be the case. Another approach has been a full calculation of the electron–solid interaction, assuming a test dielectric function, and then adjusting the test function until the calculated spectrum fits the experimental one [18,19]. A new approach to separating surface excitations from bulk one in REELS has been developed, in which a REELS spectrum is decomposed into bulk and surface excitations, without any assumption on the dielectric function at the surface [20]. Tested up to now on a few metals, such an approach to REELS is very promising, because in principle it allows one to derive the surface energy loss function from a REELS spectrum, only by knowing the bulk energy loss function, but without assuming that the dielectric function is the same at the surface and in the bulk. Once the surface energy loss function is successfully separated, then a new Kramers–Kronig dispersion relationship for the surface energy loss function will be required to derive the real part of surface energy loss function based on  $\text{Im}[1/(\varepsilon(\omega) + 1)]$ , so that one can determine surficial electronic structure and physical properties of the film materials. This Kramers–Kronig dispersion relationship for the surface energy loss function will be an welcome addition to the Kramers–Kronig dispersion relations already used in bulk (VUV reflectance) and interfacial (TEELS in the TEM) electronic structure studies [8,9].

Here we present a new effort, where we have developed a previously unreported surface Kramers–Kronig dispersion relationship for the surface energy loss function to derive the real part of  $[1/(\varepsilon(\omega) + 1)]$  and then the complex dielectric function  $\varepsilon(\omega)$ . The new KK dispersion relationship is directly applicable to very low energy REELS spectra, based on the assumption that one can derive a pure surface energy loss function from experimental REELS spectrum at very low energy, a task that we are also currently pursuing. We then would use Kramers–Kronig analysis upon this surface energy loss function to derive the conjugate part of the surface loss function and subsequently, the complex dielectric functions and optical constants. That means the electronic structure and physical properties of surficial films would be determined from REELS spectrum through the new surface KK transform, assuming that pure surface energy loss function could be separated from the bulk one in the REELS spectrum. The result would be a good approximation of the dielectric func-

tion of surficial film whose thickness is less than the inelastic mean free path (IMPF) of the electrons in REELS, in the case that it is not suitable to be probed by TEELS or optical spectroscopy, because those spectroscopies may bring more information from the bulk substrates than from the surficial films.

## 2. Surface Kramers–Kronig dispersion relationship for the surface energy loss function and test of validity

The new Kramers–Kronig dispersion relationship for the transformation of surface energy loss function is expressed in the following equations:

$$\operatorname{Re} \left[ \frac{1}{\varepsilon(\omega) + 1} \right] - \frac{1}{2} = -\frac{2}{\pi} P \int_0^\infty \operatorname{Im} \left[ \frac{-1}{\varepsilon(\omega') + 1} \right] \times \frac{\omega'}{\omega'^2 - \omega^2} d\omega' \quad (4)$$

$$\operatorname{Im} \left[ \frac{-1}{\varepsilon(\omega) + 1} \right] = \omega \frac{2}{\pi} P \int_0^\infty \frac{\operatorname{Re}[1/\varepsilon(\omega') + 1] - (1/2)}{\omega'^2 - \omega^2} d\omega' \quad (5)$$

The input surface energy loss function may be scaled according to a similar index sum rule that is comparable to the bulk index sum rule in Eq. (3). The surface index sum rule is:

$$\frac{1}{2} - \operatorname{Re} \left[ \frac{1}{\varepsilon(0) + 1} \right] = \frac{2}{\pi} \int \operatorname{Im} \left[ \frac{-1}{\varepsilon(\omega) + 1} \right] \frac{d\omega}{\omega} = \frac{2}{\pi} \int [\text{Scale\_factor} \times \text{data}] \frac{d\omega}{\omega}. \quad (6)$$

The complex dielectric function  $\varepsilon(\omega)$  is then easily obtained from  $\operatorname{Re}[-1/(1 + \varepsilon(\omega))]$  and  $\operatorname{Im}[-1/(1 + \varepsilon(\omega))]$  parts as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (7)$$

$$\varepsilon_1(\omega) + 1 = \frac{-\operatorname{Re}[-1/(1 + \varepsilon(\omega))]}{\{\operatorname{Re}[-1/(1 + \varepsilon(\omega))]\}^2 + \{\operatorname{Im}[-1/(1 + \varepsilon(\omega))]\}^2} \quad (8)$$

$$\varepsilon_2(\omega) + 1 = \frac{\operatorname{Im}[-1/(1 + \varepsilon(\omega))]}{\{\operatorname{Re}[-1/(1 + \varepsilon(\omega))]\}^2 + \{\operatorname{Im}[-1/(1 + \varepsilon(\omega))]\}^2} \quad (9)$$

In previous work, the conventional Kramers–Kronig relationship based on the bulk energy loss function has been used in processing REELS data. Surface contributions were either ignored, or subtracted after using bootstrap methods to derive the surface ELF. However, when the primary electron energy is low enough (20–200 eV), the mean free path of the electrons is very short and the surface ELF will be the significant part of the measured signal in REELS. In this case, the

new surface KK relationship can lead to a better approximation of the dielectric functions of surficial thin films from the surface energy loss function in REELS than the bulk KK relationship will. For higher primary electron energies, contributions from both bulk and surface energy loss functions should be considered, and the key issue would be separation of the surface excitation from bulk one in REELS. Assuming that the surface energy loss function could be isolated physically from volume excitations, the new surface Kramers–Kronig transform could be applied on the surface energy loss function to derive the complex dielectric functions of the surficial films.

The validity of the new surface Kramers–Kronig relationship requires confirmation before its application to transformation of surface energy loss function in REELS. Tests of the validity of the new KK transform were carried out in two ways: (1) by using an analytically generated dielectric function from the Lorentz oscillator model; and (2) by using the complex dielectric constant data derived from measurements with photon and electron spectrometers [8,9]. In each case, the test starts with a complex dielectric constant, uses the dielectric constant to create a surface energy loss function  $\operatorname{Im}[-1/(\varepsilon + 1)]$ , transforms the surface ELF using Eq. (4) to obtain  $\operatorname{Re}[-1/(\varepsilon + 1)]$ , and finally uses the two conjugate surface ELF functions to recreate the complex dielectric constant by Eqs. (8) and (9). The validity test then consists of a comparison between the original and final derived complex dielectric functions.

### 2.1. Test with Lorentz oscillator model

A complex dielectric function was created using a Lorentz oscillator model. The Lorentz model consisted of three oscillators positioned at 10, 12, and 18 eV, with widths of 3, 2, and 9 eV respectively. The relative strengths of these oscillators were 0.1, 0.1, and 0.8. Absolute scaling was obtained by requiring that the plasma frequency be 18 eV.

The complex dielectric constant for a sum of Lorentz oscillators has the form [21]:

$$\varepsilon_1 + i\varepsilon_2 = 1 + \frac{4\pi e^2}{m} \sum_{j=1}^3 \frac{N_j}{(\omega_j^2 - \omega^2) - i\Gamma_j\omega} \quad (10)$$

The real ( $\varepsilon_1$ ) and imaginary ( $\varepsilon_2$ ) dielectric components of a Lorentz test function were computed in the energy range from 2 eV to 30 eV, representing a typical experimental energy range from the visible to the VUV. A surface energy loss function ( $\operatorname{Im}[-1/(1 + \varepsilon)]$ ), and a bulk energy loss function  $\operatorname{Im}[-1/\varepsilon]$ , generated from the Lorentz oscillator dielectric function ( $\varepsilon_1$  and  $\varepsilon_2$ ), are shown in Fig. 1.

The interband transition strength ( $J_{cv}(E)$ ), is an alternate representation of the optical response of a material, and more easily displays the valence to conduction band transitions of the interband electronic structure. The  $J_{cv}(E)$ , which is related

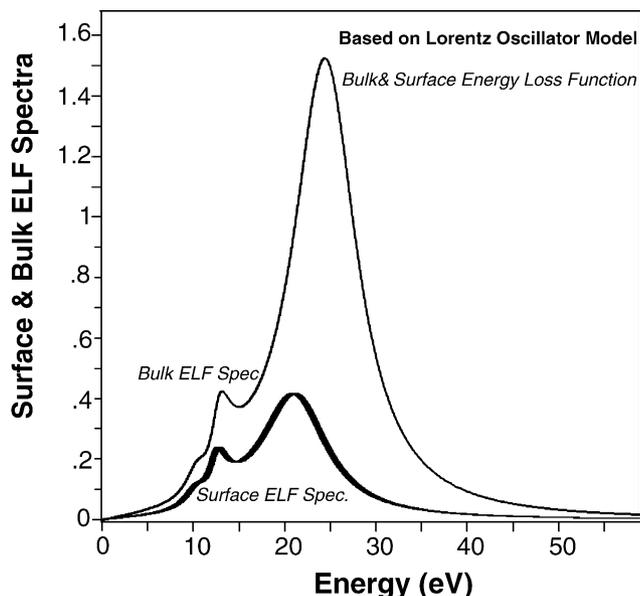


Fig. 1. Bulk and surface energy loss function generated from 3 oscillator Lorentz model.

to  $\varepsilon(\omega)$ , is expressed by

$$J_{cv}(E) = \frac{m_0^2}{e^2 \hbar^2} \frac{E^2}{8\pi^2} (\varepsilon_2(E) + i\varepsilon_1(E)) \quad (11)$$

The interband transition strength  $J_{cv}(E)$  is proportional to the transition probability and has units of  $\text{g cm}^{-3}$ . The real part of the interband transition strength for the Lorentz oscillator model,  $\text{Re}[J_{cv}]$ , is shown in Fig. 2. For computational convenience, the prefactor  $m_0^2 e^{-2} \hbar^{-2}$  in Eq. (11),

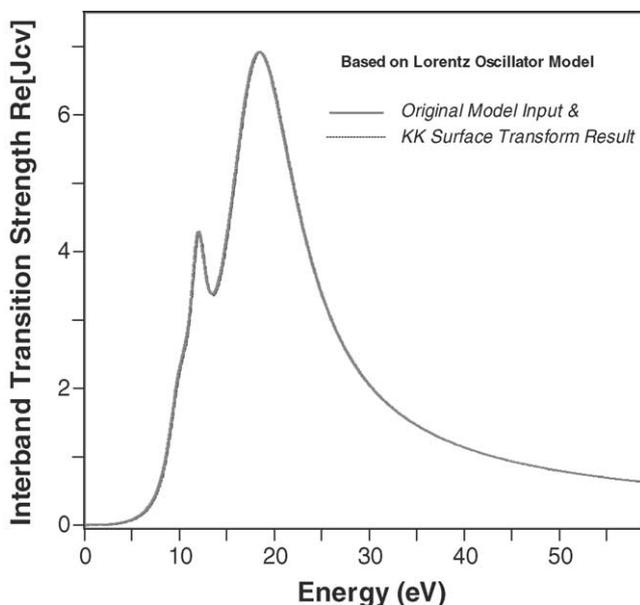


Fig. 2. Comparison of  $J_{cv}$  (interband transition strength) spectrum derived directly from Lorentz oscillator model with  $J_{cv}$  obtained using output of Kramers–Kronig surface transform.

whose value in cgs-units is  $8.289 \times 10^{-6} \text{ g cm}^{-3} \text{ eV}^{-2}$ , was taken as unity, yielding  $J_{cv}$  in units of  $\text{eV}^2$ .

The surface energy loss served as input to a computer program that performs both surface and bulk KK transforms [22]. All Kramers–Kronig transforms are defined for data that spans the energy range between 0 and infinity. The computer program used for KK analysis appends exponential wings onto the low- and high-energy ends of experimental data in order to meet this requirement. The low-energy wing for an ELF transform is formed using the functional form  $E^1$ ; the high-energy wing for an ELF transform is formed using  $E^{-3}$ . Normally, an experimental ELF is not properly scaled for KK transforms; scaling is accomplished using the index of refraction of the material in either Eq. (3) or Eq. (6). However, a Lorentz oscillator ELF generated using Eq. (10) is properly scaled, and so no scaling was applied.

After the surface KK transform to obtain the conjugate ELF,  $\text{Re}[1/(1 + \varepsilon)]$ , the program computes: (a) the complex dielectric function; (b) properly scaled, complex bulk energy loss functions; (c) properly scaled, complex surface energy loss functions; and (d) the complex interband transition strength.

A post-transform dielectric function, and post-transform interband transition strength, for the Lorentz oscillator model were thus derived from KK analysis of the surface energy loss function of the Lorentz oscillator model.

The post-transform bulk energy loss function  $\text{Im}[-1/\varepsilon]$  and surface energy loss function  $\text{Im}[-1/(1 + \varepsilon)]$  are exhibited in Fig. 1, and superimpose on the original energy loss functions calculated directly from the oscillator model. As expected the surface plasmon energy is at lower energy than the bulk plasmon energy and the surface loss intensity is lower than that of the bulk loss function. The post-transform  $J_{cv}$  function perfectly matches the  $J_{cv}$  calculated directly from the Lorentz oscillator model, as shown in Fig. 2.

### 2.2. Test of surface KK relationship on SrTiO<sub>3</sub>

The preceding self-consistency test of the new proposed surface Kramers–Kronig dispersion relationship is repeated using available complex dielectric functions of SrTiO<sub>3</sub> [8,9]. The complex dielectric function of SrTiO<sub>3</sub> was obtained from transmission electron energy loss spectroscopy (TEELS). Fourier Log Deconvolution was performed on the experimental TEELS spectra to remove the multiple scattering, giving the single scattering bulk energy loss function for SrTiO<sub>3</sub>. The bulk energy loss function  $\text{Im}[-1/\varepsilon]$ , obtained after scaling with the index sum rule on the single scattering energy loss spectrum, is shown in Fig. 3 as a black line. In this way, the complex dielectric function of SrTiO<sub>3</sub> can be generated through Kramers–Kronig transform of the bulk energy loss function. Then the surface energy loss function was calculated using the generated complex dielectric functions from TEELS. The calculated surface energy loss function of SrTiO<sub>3</sub> is shown in Fig. 3 as a gray line. Once

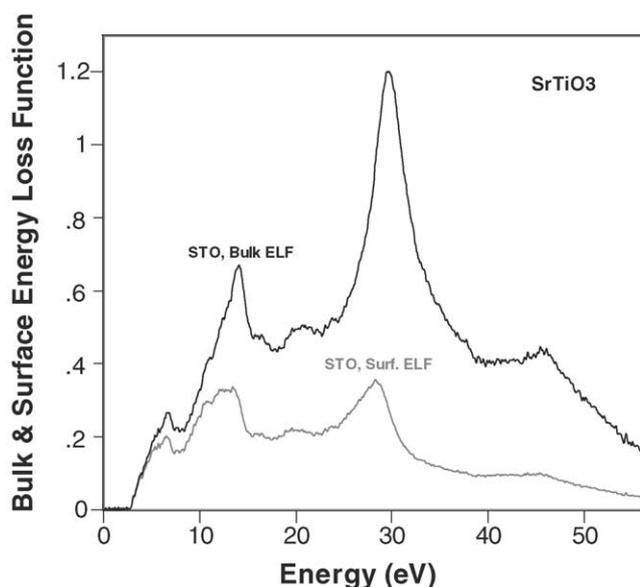


Fig. 3. Comparison of bulk ELF derived from TEELS data for SrTiO<sub>3</sub>, and surface ELF derived through bulk KK transform of the TEELS data, with the bulk and surface energy loss functions derived from application of the new surface KK transform to the surface ELF. The traces are superimposed.

the surface energy loss function was generated, the surface Kramers–Kronig dispersion relationship of Eq. (4) was then applied on the surface ELF to obtain  $\text{Re}[-1/(\epsilon + 1)]$ , from which the complex dielectric function ( $\epsilon_1 + i\epsilon_2$ ) could be calculated through Eqs. (8) and (9). After the complex dielectric function was obtained from the new surface KK transform of the surface energy loss function, the interband transition strength spectrum ( $J_{cv}$ ) of SrTiO<sub>3</sub> was then calculated using Eq. (11). The  $J_{cv}$  spectrum from the post-transform of surface ELF is shown in Fig. 4 as a dotted line. As a complex

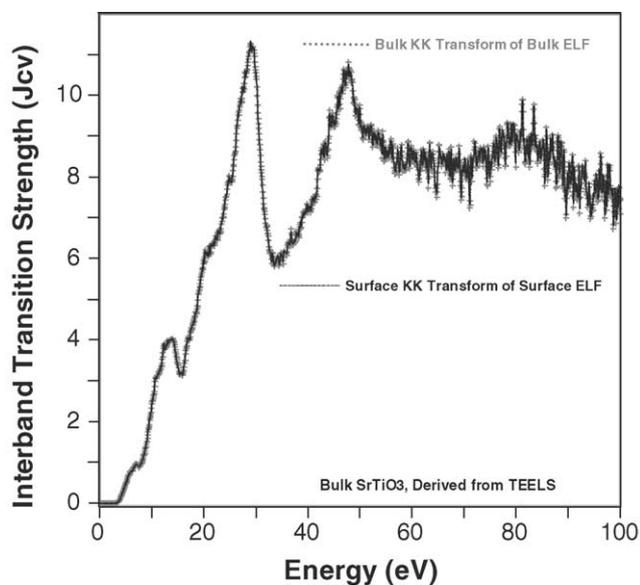


Fig. 4. Comparison of the interband transition strength ( $J_{cv}$ ) for SrTiO<sub>3</sub>, obtained by KK analysis of the TEELS data, with the  $J_{cv}$  computed from application of the newly developed KK transform to surface ELF of Fig. 3.

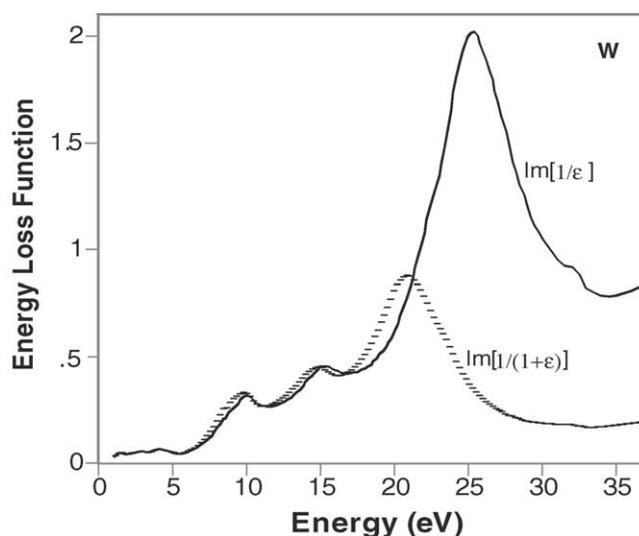


Fig. 5. Bulk and surface energy loss function of tungsten, being calculated from optical constant of W in [23].

dielectric function derived from the conventional bulk KK transform of the TEELS SrTiO<sub>3</sub> data was already available, this complex pair was also input into Eq. (11) to calculate an interband transition strength ( $J_{cv2}$ ); the result is also exhibited in Fig. 4 as solid line. It's easily seen that both the interband transition strength spectrum through conventional KK transform of bulk energy loss function and the interband transition strength spectrum through surface KK transform of surface energy loss function overlap each other; no significant difference in traces is discernable.

### 2.3. Test of surface KK upon metal tungsten

The plasma resonances in insulators, i.e. SrTiO<sub>3</sub>, are associated with the collective oscillation of the the electrons in the valence band [21]. In metals, the plasma resonances are associated with the collective oscillations of the free electron gas near the Fermi surface, which is excited by the long-range Coulomb interactions [21]. The plasma resonances of free electron gas in metals behave in a much stronger way than that of bounded electrons in valence band of insulators, the physical pattern of plasmon resonance is very clear for free electron metals. Therefore, it's helpful to take a test of surface KK transformation upon surface energy loss function of transition metal tungsten.

The plasma resonance spectra of metal tungsten, in the form of energy loss spectra, were calculated from its complex dielectric function, which was determined from the optical constants of W [23]. The probability for a surface or bulk plasma is given by the respective loss function,  $\text{Im}[-1/(\epsilon + 1)]$  and  $\text{Im}[-1/(\epsilon)]$ . Once the complex dielectric function of metal tungsten was obtained, then post-transform bulk and surface energy loss functions were calculated. Both the bulk and surface energy loss function of meal tungsten were shown in Fig. 5, where  $\text{Im}[-1/(\epsilon)]$  is the bulk energy

loss function and  $\text{Im}[-1/(\varepsilon + 1)]$  is the surface energy loss function. The dominant feature in the bulk energy loss function is a maximum at 25.3 eV, which is comparable to the calculated free electron plasma energy at 22.82 eV [24]. The surface plasmon peak, which one might expect to occur in a free electron metal, at roughly  $22.82/\sqrt{2} = 16.1$  eV, actually appear at 20.8 eV in Fig. 5. Since there is considerable interband activity near 25 eV and 16 eV, it is not surprising that the energy is shifted from the value of free electron model [24]. Similar large deviation of the plasmon resonance from the theoretical value in free electron model has also been observed in other transition metals [25,26]. Two additional pairs of features appear in the energy loss functions of Fig. 5 at energies of 10.0 eV and 9.7 eV for one pair as well as 15.2 eV and 14.8 eV for the other, respectively. The pair peaks at higher energies can be also identified as bulk plasmon while that at lower energies correspond to surface plasmon. Like the other transition metals of Nb, Mo, and Ta [25,26], in view of W loss function, it seems that each of bcc transition metals has three bulk and three surface plasmons.

After the surface energy loss function was generated, the surface Kramers–Kronig dispersion relationship of Eq. (4) was then applied on the surface ELF to determine  $\text{Re}[-1/(\varepsilon + 1)]$ , from which the post-complex dielectric function ( $\varepsilon_1 + i\varepsilon_2$ ) could be calculated through Eqs. (8) and (9). After the complex dielectric function was obtained from the new surface KK transform of the surface energy loss function, the interband transition strength spectrum ( $J_{cv}$ ) of W was then calculated using Eq. (11), the result of which is shown in Fig. 6 as dash line. Meanwhile, the interband transition strength spectrum has been also determined directly from the original complex dielectric function of metal tung-

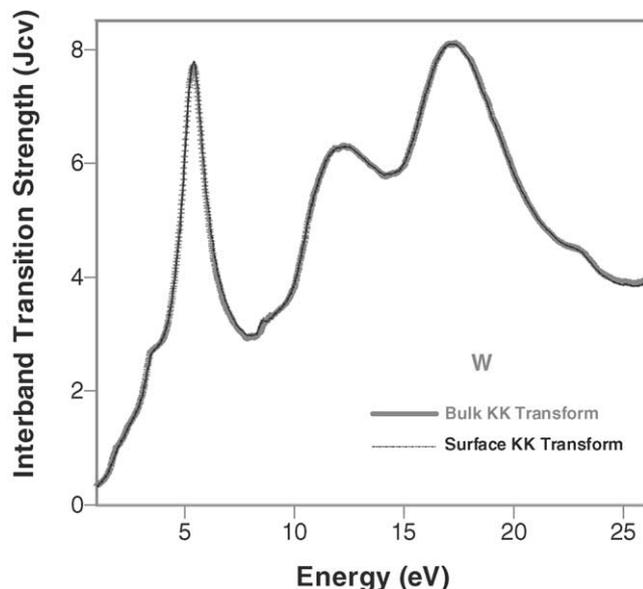


Fig. 6. Comparison of interband transition strength spectrum ( $J_{cv}$ ) of W, one was calculated from bulk KK transformation of bulk energy loss function of W, the other one was calculated from surface KK transformation of surface energy loss function of W. Both  $J_{cv}$  spectra superimposed together.

sten, which was calculated from available optical constants in Handbook [23]. This result has also been shown in Fig. 6 as a gray coarse line. It is easily seen that both pre- and post-interband transition strength spectra in Fig. 6 superimpose together. Small differences that are occurred in the round-robin comparison test are magnified by the  $E^2$  factor of Eq. (11). Nonetheless, the good agreement between the original traces and post-surface KK transform traces displayed in Fig. 4 and Fig. 6 provides assurance that the new surface Kramers–Kronig dispersion relationship in Eqs. (4) and (5) is valid for the transformation of surface energy loss function.

### 3. Conclusions

We have developed a new pair of Kramers–Kronig (KK) dispersion relationships for the surface energy loss function  $\text{Im}[-1/(1 + \varepsilon)]$  which permit Kramers–Kronig analysis to determine the complex dielectric function as well as complex optical properties. The validity of this new Kramers–Kronig relationship has been successfully confirmed by using an analytically generated dielectric function from a Lorentz model, and dielectric functions of insulator  $\text{SrTiO}_3$  and of the transition metal tungsten. For the insulator  $\text{SrTiO}_3$ , the complex dielectric function was derived from the conventional KK transform of the bulk energy loss function determined from TEELS spectra. For the transition metal tungsten, the complex dielectric function was calculated from the available optical constants. Then these original complex dielectric functions were used in two ways, one was directly for the calculation of the interband transition strength spectrum ( $J_{cv}$ ), the other one was for the derivation of surface energy loss function  $\text{Im}[-1/(1 + \varepsilon)]$ , which was then transformed by the new surface KK relationship back into post-KK complex dielectric functions. The post-KK interband transition strength ( $J_{cv}$ ) was then calculated from these post-KK dielectric functions. The original  $J_{cv}$  spectrum and post-KK  $J_{cv}$  spectrum matched very well for both the insulator and the transition metal, indicating the validity of the new surface Kramers–Kronig dispersion relationship for the transformation of surface energy loss function.

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