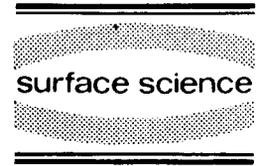




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Theory of surface electromigration on metals:
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Abstract

We present a calculation of the force, due to electron scattering, acting upon an adatom at the surface of a current-carrying metal, i.e., the so-called “wind” force in surface electromigration. The force is calculated from the Feynman–Hellmann theorem in which the electron scattering states are computed with full multiple scattering corrections by a layer-KKR method. In contrast to previous jellium models, this approach allows the proper treatment of electron scattering by both the surface barrier and the substrate and its effect upon the current-carrying states at the surface. The electron scattering force is computed for the self-electromigration of Cu adatoms on Cu(111). At room temperature, the effective valence of the adatom is found to be ≈ -21 . We conclude that surface electromigration of Cu on Cu(111) is dominated by the electron scattering force and that any direct force originating from charge transfer to the adatom is likely to be unimportant in this case. The implications of the computed value of the wind force for the mass transport at a current-carrying metal surface are discussed.

When an electrical current flows through a material, the migration of atoms results. This phenomenon, called electromigration, is of considerable technological interest because it has been implicated as a major cause of interconnect failure in integrated circuits [1]. Recently, there have been a number of experimental observations of electromigration at surfaces [2]. While the majority of these observations are of electromigration at semiconductor surfaces, there do exist several experimental studies of self-electromigration on metals [3]. In this paper we obtain a

quantitative theoretical description of the driving force for the surface electromigration of an adatom on a current-carrying metallic substrate.

Compared to surface electromigration, electromigration through bulk materials is a relatively well understood phenomenon [1]. The force acting on an atom embedded in a current-carrying host is often written as the sum of two terms,

$$F = e(Z_d + Z_w)E, \quad (1)$$

where E is the applied electric field. The first term in Eq. (1) represents the so-called “direct” force that is associated with the direct electrostatic interaction between the applied electric field and effective valence of the ion, Z_d , although the theoretical description of the direct

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component of the driving force is characterized by conceptual uncertainties [4]. The second term in Eq. (1), which is usually the dominant driving force for bulk electromigration in metals, represents the electron “wind” or scattering force produced by the electron current impinging upon the migrating atom. According to a simple ballistic model of a free-electron metal, this contribution to the total force would be equal to the rate of momentum transfer from the moving electrons to the atom. Therefore, the effective valence associated with the wind force, Z_w , is a function of the current flowing in the sample. For bulk electromigration, the wind force has been calculated for impurities in bulk free-electron [5,6], noble and transition metals [7–9], mesoscopic metallic superlattices [10] and thin films [11].

To our knowledge, there have been two attempts to develop theoretical models of surface electromigration, both based upon the simple ballistic method embodied in the Huntington–Grone–Fiks model [5,12]. Sorbello and coworkers [13] have calculated the wind force acting on a point impurity located inside the surface of a free-electron metal. The surface was represented by an infinite potential barrier. Duryea and Huntington [14] have calculated the wind force for self-migration of a sodium atom embedded in a (finite-barrier) jellium surface. The latter results were sensitive to the potential chosen for the sodium atom but indicated that a sodium atom close to the jellium surface experiences a wind force that is similar in magnitude to its value in the bulk.

In this paper we present a theory of surface electromigration based upon a layer-KKR technique. Previously, the layer-KKR method has been applied to the calculation of several bulk and interface properties. These applications include the magnetic and electronic properties of metallic superlattices [15], monolayer magnetism in transition metals [16], the electronic, magnetic and mechanical properties of planar faults in elemental metals [17], ordered [18] and disordered alloys [19], local magnetic moments of impurities in alkali metals [20], cohesive energies of stacking faults [17] and grain boundaries [21], resonance electron scattering by molecules ad-

sorbed on metallic substrates [22], and the calculation of low-energy electron diffraction spectra [23].

In this work, the layer-KKR technique is applied to the calculation of the wind force in surface electromigration on metals in which the electron scattering states are computed within the muffin-tin approximation and the force is calculated from the Feynman–Hellmann theorem. In contrast to calculations based upon the jellium model, this approach allows both the electronic structure of the substrate/adatom system and the influence the surface barrier to be fully incorporated. Consequently, this method is not confined to simple metals, but may be used to obtain quantitative estimates of the wind force for surface electromigration on, for example, transition and noble metals.

To calculate the driving force acting upon an adatom situated on the surface of a metal through which a current flows, we employ a generalization of bulk KKR methods which have been applied to bulk electromigration by Gupta [11] and van Ek and Lodder [9]. A more detailed presentation of the theory outlined here will be set out in a subsequent publication. Within the Born–Oppenheimer approximation the force is

$$F = - \sum_k g(\mathbf{k}) \langle \psi_k | \nabla_R V(\mathbf{r} - \mathbf{R}) | \psi_k \rangle, \quad (2)$$

where ψ_k is an electronic wavefunction of the adatom/surface system with wave vector \mathbf{k} , $V(\mathbf{r})$ is the atomic potential of the adatom located at \mathbf{R} , and \mathbf{r} is the electronic coordinate. In atomic units, the population of the scattering states caused by the applied electric field is described by the distribution function

$$g(\mathbf{k}) = -(\mathbf{v}_F(\mathbf{k}) \cdot \mathbf{E}) \tau \delta(\mathcal{E} - \mathcal{E}_F), \quad (3)$$

where \mathbf{v}_F is the Fermi velocity, \mathcal{E}_F is the Fermi energy, and τ is the average relaxation time at the surface which we assume to be independent of $\hat{\mathbf{k}}$.

For the surface electromigration of an adatom, the wind force is anisotropic and dependent upon the location of the adatom within the surface unit cell. Therefore, the effective valence of the mi-

grating adatom must be represented by a 2×2 tensor \mathbf{Z}_w such that

$$F = \mathbf{Z}_w(\mathbf{R})E. \quad (4)$$

When expressed with respect to an origin at the adatom, the surface electronic states can be expanded in spherical harmonics

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{4\pi}{\sqrt{\Omega}} \sum_{lm} i^l A_{lm}(\mathbf{k}) R_l(r) Y_{lm}(\hat{\mathbf{r}}), \quad (5)$$

where R_l is a radial solution of the Schrödinger equation and Ω is the volume of the substrate unit cell. In terms of these spherical wave coefficients, A_{lm} , the wind force is obtained by integrating over the shifted Fermi sphere. The components of the (Cartesian) effective valence tensor are [24]:

$$(Z_w)_{ij} = 4\tau \sqrt{\frac{2}{\pi}} \int_{\text{FS}} \frac{d^2\mathbf{k}}{|\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}|} (\nu_{\text{F}}(\mathbf{k}) \cdot \hat{\mathbf{x}}_j) I_i(\mathbf{k}), \quad (6)$$

$(i, j) = x, y,$

where

$$I_i(\mathbf{k}) = + \sum_{lm} \sum_{l' = l \pm 1} \sum_{m' = m \pm 1} (-1)^m A_{lm}^* A_{l'm'} \times \sin^2(\delta_l^a - \delta_{l'}^a) B_i(lm, l'm'), \quad (7)$$

and

$$B_x(lm, l'm') = (C_{l,-m;l',m';1,-1} - C_{l,-m;l',m';1,1}),$$

$$B_y(lm, l'm') = i(C_{l,-m;l',m';1,-1} + C_{l,-m;l',m';1,1}),$$

where the δ_l^a 's are the phase shifts of the adatom and the C 's are Gaunt coefficients.

Within the muffin-tin approximation, Eq. (6) is a general expression for the electron scattering force experienced, at $T = 0$ K, by an adatom on a current-carrying substrate. The coefficients of the spherical wave expansion, A_{lm} , are obtained from the calculated surface electronic wavefunctions in the vicinity of the adatom. The electron scattering states $\psi_{\mathbf{k}}$ are evaluated by numerically integrating the Schrödinger equation through the surface barrier region and then satisfying the continuity condition at the first atomic plane of the substrate. The boundary conditions to be satisfied at this matching plane are determined from the reflection matrix, R_S , of the substrate, which is evaluated using a layer-KKR theory.

In keeping with other layer-KKR-based multiple scattering theories [25,27], the potential of both the adatom and the substrate atoms was of a muffin-tin form, immersed in a constant interstitial potential. After determining the atomic phase shifts, the scattering paths within one atomic layer parallel to the surface are summed using the Kambe method [28]. The atomic planes are then assembled into the semi-infinite, bulk-terminated surface using the layer-doubling algorithm [27] to sum the interlayer multiple-scattering paths [29]. A full description of the theory of the layer-KKR method [25], its computational implementation [26] and its generalization to surface problems may be found elsewhere [22,23].

In the numerical implementation of this approach, we used angular momenta up to $l_{\text{max}} = 3$ for the substrate layer-KKR calculation. The sum over the spherical wave amplitudes required to evaluate the force (Eq. (7)) was truncated at $(l, l') \leq l_{\text{max}} + 1$. The plane-wave basis set contained up to 21 reciprocal lattice vectors. The integral over the two-dimensional Brillouin zone was performed using the method of special points [30]; several hundred sampling points within the irreducible wedge of the surface Brillouin zone were included. For the surface barrier, we employed the saturated image potential model of Jones et al. [31] with parameters fitted to the binding energy of image states by Smith and coworkers [32].

As a first application of this approach, the electron scattering force for self-electromigration of an isolated Cu adatom on Cu(111) was computed. The potential for both the substrate atoms and adatom was determined by a self-consistent field, layer-KKR calculation for bulk Cu [26]. This potential has been shown to reproduce the electronic structure of bulk Cu and has been used to determine the local electronic states at low-coordination, planar stacking faults in Cu [26,33].

In Fig. 1 the computed electron scattering forces, both in the direction of the applied field E and perpendicular to E , are displayed as a function of the lateral position of the adatom. E was applied parallel to the surface in the $[1\bar{1}0]$ direction, and the wind force is computed along the contour (shown in Fig. 2) which links the

preferred fcc-hollow binding sites *via* the bridge and hcp-hollow sites. This contour includes segments of the preferred migration pathways for adatom transport parallel to the $[1\bar{1}0]$ and $[11\bar{2}]$ directions. The actual migration pathways were determined by computing the adatom binding energy as a function of the lateral position by the embedded-atom-method (EAM) [34]. EAM calculations were also employed to determine the height the adatom above the first atomic plane of the substrate as a function of position of the adatom in the surface unit cell [35].

In order to remove the temperature dependence of the substrate resistivity, the components of the wind force are expressed as the ratio of the effective valence to the average relaxation time: Z_w/τ . As can be seen from Fig. 1, the component of the wind force parallel to the applied field is

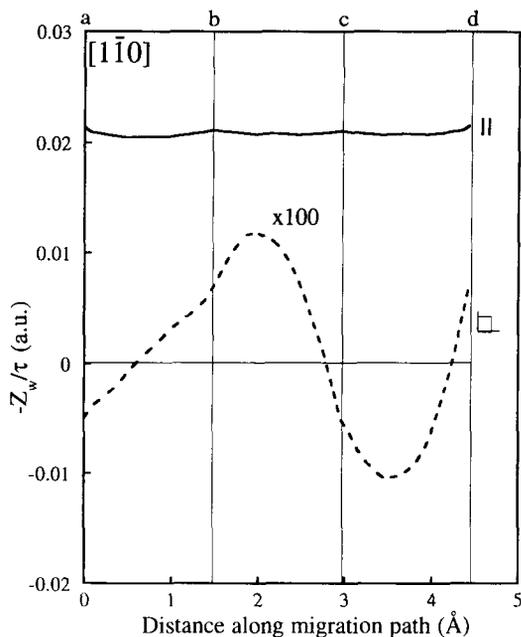


Fig. 1. The wind force acting upon a Cu adatom on a Cu(111) surface, plotted as a function of the lateral position of the adatom. The applied electric field is in the $[1\bar{1}0]$ direction. The wind force is expressed as the ratio of the effective valence to the relaxation time expressed in atomic units; at 293 K, $\tau \approx 1000$ a.u.. The solid curve is the component of the wind force parallel to the field, the dashed curve is the component of the wind force perpendicular to the field. The lateral position of the adatom along the migration pathway is shown in Fig. 2.

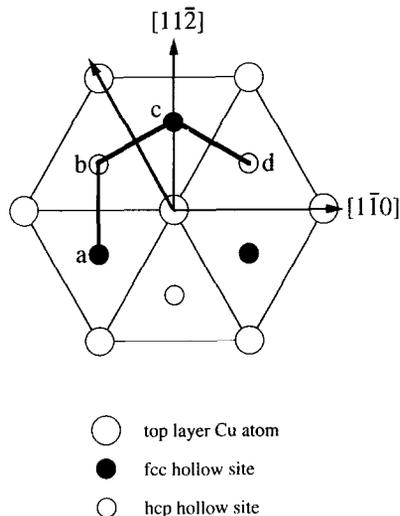


Fig. 2. A schematic illustration of a top view of the Cu(111) surface showing the top layer Cu atoms (open circles) and the fcc-hollow and hcp-hollow sites. The contour along which the wind force is calculated is shown as the solid line abcd. The adatom positions labelled a and c are fcc-hollow sites and the positions b and d are hcp-hollow sites.

almost two orders of magnitude greater than the perpendicular component. Therefore the wind force acts almost parallel to the direction of the applied field. The magnitude of the wind force is found to be almost independent of the lateral position of the adatom within the unit cell. The magnitude of the wind force, averaged over the migration pathway for this field direction (cdcd...), is $Z_w/\tau = -0.0208$ (a.u.). At room temperature we can estimate the magnitude of the wind valence by using the bulk average relaxation time, $\tau \approx 1030$ (a.u.), so that the average effective valence of the adatom is $Z_w = -21.4$ when the electric field is applied in the $[1\bar{1}0]$ direction. The negative sign of the average effective valence indicates that the force acts in the same direction as that of the electron flow (i.e. towards the anode).

Fig. 3 displays both components of the computed electron scattering force when E is applied in the $[11\bar{2}]$ direction (see Fig. 2). In this case, the field is applied in an (inequivalent) direction perpendicular to the field employed in Fig. 1. Comparing the forces shown in Figs. 1 and 2, it is apparent the magnitude of the wind force is

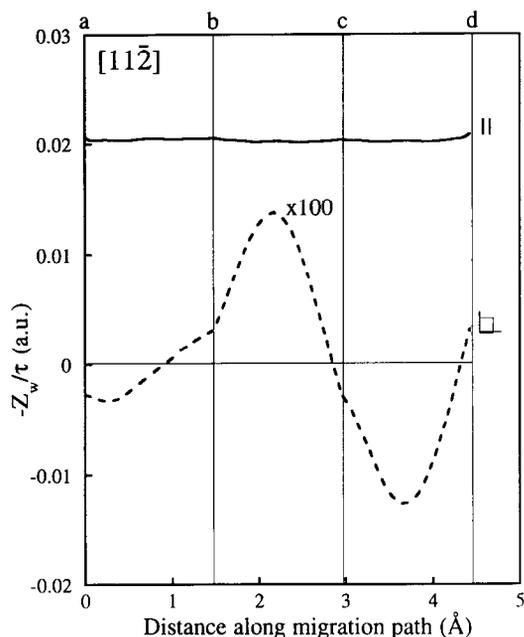


Fig. 3. Same as Fig. 1, but for an applied electric field which is in the $[11\bar{2}]$ direction.

almost independent of, and parallel to, the direction of the applied field: At room temperature, the effective valence averaged over the migration path (abcb...) is -20.9 when the field is applied along the $[11\bar{2}]$ direction compared to -21.4 when the field is applied parallel to the $[1\bar{1}0]$ direction. Given the similarity of these computed values of Z_w and the relatively small magnitude of the components of the wind force perpendicular to the field, the wind force for Cu surface self-electromigration is evidently almost isotropic [36]. These results also indicate that, at room temperature, the dominant driving force for self-electromigration of Cu adatoms on Cu(111) is the wind force (i.e. $|Z_w| \gg 1$); the direct force (if any) makes a relatively small contribution to the total driving force.

The calculated values of Z_w for surface self-electromigration on Cu(111) may be compared to the wind force for bulk self-electromigration in Cu calculated by Gupta [11]. Using a multiple-scattering method, Gupta finds the effective va-

lence for bulk electromigration to be $Z_w = -3.2$ at 1000°C . Using the quoted temperature dependence of the resistivity [37], Gupta's calculation predicts an effective valence of $Z_w = -15.8$ at 293 K . This value is similar to our calculated value of the effective valence for surface electromigration, $Z_w \approx -21$. However, it should be noted that the wind valence for surface electromigration is proportional to the average relaxation time at the surface and this quantity may differ, perhaps significantly, from the bulk value we have used to compute Z_w for the adatom [38]. Nevertheless, this comparison suggests that the wind force acting upon a Cu adatom is similar in magnitude to the wind force experienced by a Cu atom migrating through the bulk. Another calculation of bulk electromigration of interstitial Cu employs a pseudopotential method and finds the ratio of the wind force to the current density to be $F/j = 249 \times 10^{-6} \text{ eV cm}^{-1} \text{ A}^{-1}$ [39]. This value is substantially larger than both Gupta's result for bulk (substitutional) migration and our value for the wind force for surface electromigration which, in this set of units, are $F/j = 27 \times 10^{-6} \text{ eV cm}^{-1} \text{ A}^{-1}$ and $F/j = 34 \times 10^{-6} \text{ eV cm}^{-1} \text{ A}^{-1}$, respectively. The only other quantitative calculation of the wind force in surface electromigration is the jellium calculation for Na self electromigration performed by Duryea and Huntington [14]. They find the wind force to be in the range $F/j = (56-89) \times 10^{-6} \text{ eV cm}^{-1} \text{ A}^{-1}$ or $-8.6 \geq Z_w \geq -13.8$ at 85°C . This result is similar in magnitude to the wind force we have computed for adatom migration on Cu(111).

To our knowledge the only experimental studies of adatom electromigration at metallic surfaces are of Ni migration over polycrystalline W and Mo surfaces [3]. In these studies it was found that the adatom migrated towards the anode under the action of the wind force with an effective valences of $-0.4 \geq Z_w \geq -2.6$ and $-0.5 \geq Z_w \geq -3.1$, respectively, at elevated temperatures of $900-1000^\circ\text{C}$. At 293 K , the corresponding values are $-1.7 \geq Z_w \geq -11.1$ for the W surface and $-2.2 \geq Z_w \geq -13.3$ for Mo, after correcting for the temperature dependence of the resistivity. Therefore, the limited experimental data on surface electromigration at metallic surfaces appears

to be consistent with the qualitative nature of the driving force obtained in this paper for Cu self-electromigration, in particular, the dominance of the wind force.

The results obtained by the layer-KKR method show that the electromigration of Cu adatoms on Cu(111) is qualitatively similar to that expected for bulk electromigration in a free-electron metal in which the wind force is parallel to the applied field and the effective valence is isotropic. Therefore, it is instructive to compare the computed forces to a ballistic calculation in which the force is equal to the rate of momentum transfer from the conduction electrons [12,40]. According to this simple model, $Z_w = -n_0 l \sigma_{tr}$ where n_0 is the electron concentration (for bulk Cu, $n_0 = 8.45 \times 10^{-2} \text{ \AA}^{-3}$ [41]), l is the mean free path ($l = 393 \text{ \AA}$ at 293 K [41]), and σ_{tr} is the transport cross section of the adatom at the Fermi energy. The transport cross section was computed from the Cu phase shifts employed in our layer-KKR calculation and found to be $\sigma_{tr} = 1.29 \text{ \AA}^2$. It follows that the ballistic value for the effective valence is $Z_w = -43.2$. Therefore, we find that the computed magnitude of the effective valence for surface self-electromigration on Cu(111), $Z_w \approx -21$, is approximately half the bulk value obtained using the ballistic model. This reduction of the calculated effective valence at the surface reflects the lower coordination of the adatom relative to the bulk, an effect which would lead to a reduction of the local carrier density, and consequently of the ballistic wind force in the surface region. We note that differences between the relaxation time at the surface of the metal and within in the bulk would also be expected to alter the relative magnitude of the wind force observed at the surface and in the bulk. However, this effect is not included in our model of Cu self-electromigration.

It should be noted that the apparent agreement between the ballistic model and the layer-KKR calculation, which includes the full band structure, is not an obvious conclusion. It is well known that the ballistic model fails to provide a quantitative description of wind force for bulk electromigration in transition and noble metals since it is applicable only within the free-electron

model [40]. Nevertheless, the agreement between the ballistic model and the layer-KKR calculation, and in particular the isotropy of the computed wind force, suggests that the low coordination of an adatom relative to a substitutional impurity in the bulk may play a role in reducing the contribution to the wind force from multiple electron scattering in the vicinity of the adatom, at least in the case of Cu self-electromigration on Cu(111).

Finally, we consider the implications of the computed wind force for mass transport of adatoms on a current-carrying metallic substrate. First, we remark that the change in the adatom binding energies of adjacent hollow sites, caused by the applied field, is on the order of 10^{-8} – 10^{-9} eV for an applied electric field of 1 mV cm^{-1} . This value may be compared to the activation barrier to diffusion for adatoms which is of the order of 0.1–1 eV for most metals surfaces. Consequently, the wind force causes only a small perturbation or bias of the activation barriers for diffusion that drives mass transport in the direction of the electronic current. In the case where mass transport is dominated by adatom diffusion, the drift velocity of the adatoms can be estimated from the Einstein relation [2]:

$$v_{\text{drift}} = \frac{D Z_w E}{k_B T}, \quad (8)$$

where T is the temperature and D is the *surface* diffusion constant. D is assumed to have the usual Arrhenius form

$$D(T) = D_0 \exp\left(-\frac{E_a}{k_B T}\right), \quad (9)$$

where E_a is the activation energy barrier for adatom diffusion in the absence of the driving force and D_0 is the pre-exponential factor. For Cu(111), according to EAM calculations [42], $D_0 \approx 3 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1}$ and $E_a \approx 0.044 \text{ eV}$, and we have found $Z_w = -21$. Consequently, at 293 K, when a current of 1 A flows, parallel to the (111) face, through a Cu sample with a cross-sectional area of 1 mm^2 , $E = 0.167 \text{ mV cm}^{-1}$, and $v_{\text{drift}} \approx 730 \text{ \AA s}^{-1}$. At elevated temperatures, the drift

velocity for Cu self-electromigration on Cu(111) is weakly temperature dependent; $v_{\text{drift}} \approx 850 \text{ \AA s}^{-1}$ at 400 K and $v_{\text{drift}} \approx 670 \text{ \AA s}^{-1}$ at 1173 K. For the more open surfaces of Cu, the activation barrier to surface diffusion is significantly larger, $E_a \approx 0.7 \text{ eV}$ for Cu(100) [42]. If it is assumed that the magnitude of the adatom wind valence for Cu(100) is similar to that computed for Cu(111), then surface self-electromigration on Cu(100) would only be significant at elevated temperatures; $v_{\text{drift}} \approx 1 \text{ \AA s}^{-1}$ at 1173 K.

In conclusion, we have performed a quantitative calculation of the electron-scattering (wind) force acting upon a Cu adatom migrating across a current-carrying Cu(111) surface. At room temperature, the wind force is parallel to the direction of the applied field and displays little variation as a function of the lateral position of the adatom. These features would also be expected from a ballistic model of electromigration at the surface of a free-electron metal. At $T = 293 \text{ K}$, the magnitude of the wind force is equivalent to an average effective valence of approximately -21 . This value is similar to that obtained for bulk electromigration in Cu and is approximately a factor of two smaller than the value obtained by a simple ballistic argument. Our result suggest that the wind force is the dominant driving force for surface self-electromigration on Cu(111). More generally, the layer-KKR approach presented in this paper offers the opportunity for detailed quantitative studies of the driving force for surface electromigration on transition and noble metals. Applications of the layer-KKR method to other adatoms and substrates will be reported in a future publication.

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- [35] The computed adatom heights from EAM were $d = 2.03$ Å for the fcc-hollow site, $d = 2.05$ Å for the hcp-hollow site and $d = 2.13$ Å for the bridge site. For comparison, the height of an adatom placed in the continuation site is 2.08 Å.
- [36] For an adatom in the fcc-hollow site, at room temperature, the components of the effective valence tensor, Z_w , are: $Z_{xx} = -22.04$, $Z_{yy} = -21.22$, $Z_{xy} = +0.05$ an $Z_{yx} = +0.03$. Since the diagonal elements are almost equal and the off-diagonal elements are almost zero, the wind force is nearly isotropic.
- [37] $\rho_0(T) = 1.673 + 0.0068(T - 293) \mu\Omega \text{ cm}$ (cf. Ref. [11]).
- [38] There is a limited body of work concerning the surface resistivity of metals. See, for example: B.N.J. Persson, Surf. Sci. 169/270 (1992) 103.
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