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Relationship between adatom-induced surface resistivity and the wind force for adatom electromigration: A layer Korringa-Kohn-Rostoker study

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An isolated adatom adsorbed onto the surface of a current-carrying metal feels an electromigration wind force and also changes in the resistivity of the surface. Using the jellium model, it is possible to derive a simple relationship between the wind force F_w and change of the surface resistivity, $\Delta\rho_s$, induced by the adatom. This relationship arises because both of these quantities have a common physical origin: the exchange of momentum between the adatom and the carriers impinging upon the surface from the interior of the metal. A layer Korringa-Kohn-Rostoker calculation is used to study the relationship between the electromigration wind force and the surface resistivity induced by an isolated Ag adatom on Ag(111). In contrast to all prior studies of adatom electromigration at surfaces, our approach permits the computation of the wind forces felt by both the adatom and by atoms within the substrate. We show that the presence of the adatom significantly alters the magnitude of the wind force exerted on substrate atoms that are close to the adatom adsorption site. We use this information to study how the momentum transfer occurring at the surface is partitioned among the adatom and the substrate atoms and show how this effect significantly alters the relationship between F_w and $\Delta\rho_s$ derived from jellium models of the substrate.

Atoms adsorbed onto the surface of a metal elastically scatter carriers impinging upon the surface from the bulk, altering their momentum parallel to the surface. Consequently, adatom adsorption changes the surface resistivity ρ_s of the metal,[1–6] a phenomenon that has been observed in measurements of the resistivity of metallic thin films.[7,8] The momentum transfer between the carriers and the surface also gives rise to forces that are localized at the surface of the metal. These forces correspond to the so-called ''wind force'' in surface electromigration, F_w.[4,9–15] The wind force induces a bias in the thermally activated diffusion of the adatoms which can give rise to significant mass transport along the surface and current-induced changes in surface morphology.[16]

Since both the electromigration wind force felt by an adatom, F_w^a, and the change in the surface resistivity it induces, $\Delta\rho_s$, have a common physical origin, it seems plausible that there should exist a simple relationship between F_w^a and $\Delta\rho_s$. An analogous relationship is well known in the theory of bulk electromigration[17–19] where a ballistic theory of electron scattering from an impurity atom in a free-electron gas allows one to derive the following relation between the residual resistivity of the impurity ρ_i and the wind force it feels, $\mathbf{F}_w$:

$$\mathbf{F}_w = -\frac{e\,\eta\rho_i}{N_i}\mathbf{J}. \tag{1}$$

Here η is the bulk carrier density, N_i is the number density of impurity atoms, and $\mathbf{J}$ is the bulk current density. Implicit in the derivation leading to Eq. (1) is the assumption that the rate of momentum transfer from the carriers is equal and opposite to the rate of momentum transfer to the impurity atom. Clearly, this assumption is valid for an impurity embedded in a free-electron metal where momentum can only be exchanged between the impurity and the conduction electrons that carry the electrical current. A careful derivation of Eq. (1) and a detailed analysis of its validity have been performed by Sorbello.[20,21]

A simple generalization of the ballistic approach to the case of adatoms on the surface of a free-electron metallic thin film leads to the following relationship between the wind force felt by the adatom and the change in the surface resistivity it induces:[4]

$$\mathbf{F}_w^a = -\frac{e\,\eta l_f\Delta\rho_s}{\eta_a}\mathbf{J}, \tag{2}$$

where l_f is the thickness of the thin film and η_a is the areal number density of adatoms. Recently, Ishida[4] derived Eq. (2) from first principles using time-dependent density functional theory to show that this expression holds true provided that the substrate is translationally invariant parallel to the surface. Consequently, the simple relationship between $\mathbf{F}_w^a$ and $\Delta\rho_s$, expressed mathematically by Eq. (2), can be shown to be valid for adatom adsorption onto a flat jellium. Physically, the requirement for translational invariance of the substrate ensures that momentum can only be exchanged between the adatom and the carriers impinging upon the surface from the bulk. Then, in the absence of the adatom, there can be no momentum transfer between the carriers and the substrate in a direction parallel to the surface. This is essentially the same assumption made in the ballistic derivation of the analogous bulk relationship [Eq. (1)].

While this assumption may be reasonable for simple metal surfaces whose electronic structure is well approximated by the jellium model, it is not clear that such a simple relationship can describe the carrier scattering at the surfaces of other real metals. Indeed, even in the absence of adsorbates, most real metal and alloy surfaces possess a finite

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surface resistivity,[5,22–24] a fact which implies that carrier scattering at such surfaces involves some momentum transfer parallel to the surface. In particular, for transition and noble metals we anticipate significant corrections to Eq. (2) arising from the strong multiple scattering of the carriers between the adatom and atoms within the substrate. Indeed, the inclusion of carrier multiple scattering between impurity and host atoms within transition and noble metals is known to be an important ingredient of the accurate description of the wind force in bulk electromigration.[21,25–28]

To proceed further we must consider the component of electromigration wind force, parallel to the surface, acting on both the adatoms and on the atoms within the substrate. Consider an isolated adatom adsorbed on the surface of a metal carrying an electrical current. By definition, the rate of momentum transfer between the carriers and the surface is directly proportional to the net surface resistivity. The change in the surface resistivity induced by the adatom is proportional to the change in the rate of momentum transfer from the carriers that occurs when the adatom is introduced onto the surface:

$$-\frac{d\Delta\mathbf{p}}{dt}=\mathbf{F}_w^a+\sum_j \delta\mathbf{F}_w^j. \tag{3}$$

Here $\mathbf{F}_w^a$ is the wind force felt by the adatom and $\delta\mathbf{F}_w^j$ is the change in the wind force exerted upon the jth substrate atom resulting from the presence of the adatom. From Eq. (3) it is apparent that, for a translationally invariant substrate, $\mathbf{F}_w^j=0$ and $\delta\mathbf{F}_w^j=0$. In this case, Eq. (3) leads directly to Eq. (2) and the change in the surface resistivity induced by the adatom is directly proportional to the wind force acting on the adatom. However, for a real metal surface, the substrate forces with and without the adatom are not the same. In general, $\delta\mathbf{F}_w^j\neq 0$ for substrate atoms that surround the adsorption site because the additional carrier scattering introduced by the adatom alters the amplitude of the carrier states impinging on each substrate atom in its vicinity. Therefore, for a real metal surface, the second term on the right-hand side of Eq. (3) does not vanish. Then the accuracy of Eq. (2) is determined by the relative magnitude of the wind force acting on the adatom and the sum of change in the forces felt by the substrate atoms that occurs as a consequence of the addition of the adatom to the surface.

In order to investigate the validity of Eq. (2) when applied to a real metal surfaces we have used a layer Korringa-Kohn-Rostoker (layer KKR) calculation to compute the wind forces felt by both the adatom and substrate atoms for the case of an isolated Ag adatom on Ag(111). This permits the direct determination of both terms appearing on the right-hand side of Eq. (3).

The layer KKR method has been applied to several fundamental problems in electron scattering theory at surfaces including the calculation of the electromigration wind force[13,14,29,30] and the surface resistivity of metals and alloys.[23,24] To calculate the driving force acting upon atoms at surface of a metal through which a current flows, we employ a generalization of the usual KKR methods that have been applied to bulk electromigration by Gupta[25] and van Ek and Lodder.[26–28] The layer KKR method constructs the scattering properties of a surface by first assembling single atoms into atomic planes which are then combined to produce a semi-infinite stack of atomic layers that represent the substrate. This semi-infinite stack of atomic planes, oriented perpendicular to the surface normal, is then combined with the surface barrier and the adatom by self-consistently solving the multiple scattering problem for carriers impinging on the surface.

Within the Born-Oppenheimer approximation the wind force acting upon a surface atom is[14]

$$\mathbf{F}_w=-\sum_k g(\mathbf{k})\langle\psi_k|\nabla_R V(\mathbf{r}-\mathbf{R})|\psi_{\mathbf{k}}\rangle, \tag{4}$$

where $\psi_{\mathbf{k}}$ is a carrier wave function of the adatom/substrate system labeled with wave vector $\mathbf{k}$,$V(\mathbf{r})$ is the effective potential of the atom located at $\mathbf{R}$, and $\mathbf{r}$ is the electronic coordinate. $g(\mathbf{k})$ is the out-of-equilibrium part of the population of carrier states that results from the application of the electric field $\mathbf{E}$. From Eq. (4) it is apparent that the evaluation of the wind force experienced by an atom requires the self-consistent calculation of the carrier states in the vicinity of the atom. This was achieved using the layer KKR method to self-consistently compute the scattering of carriers among the adatom and surface atoms, evaluated to all orders of multiple scattering. A complete presentation of the theory, applied to the calculation of the wind force felt by the adatom, can be found in an earlier publication.[14] The principal modification to that computational framework, needed to generate the results presented in this paper, was its generalization to calculate the forces acting on both the adatom and atoms within the substrate.

This method was applied to the case of an isolated Ag adatom on Ag(111). Following the usual convention, the calculated wind forces are expressed in terms of components of an effective wind valence tensor, Z_w^{ij}, where $F_w^i\equiv eZ_w^{ij}\mathbf{E}_j$ $(i,j\equiv x,y)$, and we employ the Einstein summation convention. The calculated wind valences are normalized to the carrier relaxation time τ. This representation of the force has the virtue of being temperature independent. Figure 1 is a schematic illustration of a (111) surface showing the adsorption geometry of the Ag adatom placed in the fcc, hcp, or twofold bridge sites. Figure 1 also shows the location of each substrate atom in the vicinity of the adatom and the labeling scheme $(k=1,2,3,...)$ we use to identify each substrate atom.

First, we computed the wind force felt by Ag atoms within the two outermost atomic layers of a clean Ag(111) surface (i.e., without the adsorbed Ag adatom). We express the wind force in terms of the components of the wind valence tensor, normalized to the relaxation time τ. By symmetry, the wind forces felt by atoms in the same atomic layer are identical. For atoms in the outermost atomic layer of Ag(111), the magnitude of the wind valence for forces in the direction of the applied field was found to be $Z_w^{xx}/\tau=-6.1\times10^{-3}$ a.u. and $Z_w^{yy}/\tau=-6.0\times10^{-3}$ a.u. for $\mathbf{E}$ parallel to the inequivalent $[10]$ and $[\overline{1}2]$ directions, respectively. The corresponding forces felt by atoms in the second atomic layer were $Z_w^{xx}/\tau=-6.0\times10^{-4}$ a.u. and $Z_w^{yy}/\tau=-6.0\times10^{-4}$ a.u. Of the off-diagonal elements of the wind valence tensor, Z^{xy} vanishes identically (since the corresponding field lies in a surface mirror plane) and the calculated value of Z^{yx} was found to be 3 orders of magnitude smaller than either of the

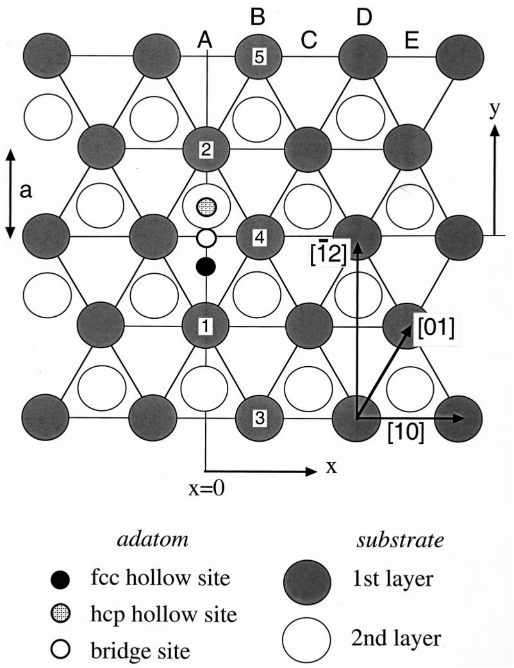

FIG. 1. A schematic illustration of the adsorption geometry of an Ag adatom on Ag(111). The Ag atoms in the first atomic layer of the substrate are indicated by large gray circles: those in the second layer are indicated as large open circles. The locations of the adatom in three high-symmetry adsorption sites are shown as small circles: the threefold fcc hollow site (small black solid circle), the threefold hcp hollow site (small shaded circle), and the twofold bridge site (small open circle). Also shown is the labeled scheme used to identify the substrate atoms in Fig. 2: a subset of Ag atoms in the top atomic layer of the substrate is numbered. Each of the substrate atoms in a layer can be identified by the row (parallel to $[\bar{1}2]$) containing it (*A*, *B*, *C*,...) and its *y* coordinate, defined relative to the fcc hollow site (at $y=0$), expressed in units of one-half of the interatomic spacing within each row.

diagonal components. Therefore, the off-diagonal components of Z_w^{ij} are negligible and are ignored in the subsequent discussion of our results. The magnitude of the wind force felt by atoms in the second atomic layer of Ag(111) is found to be approximately an order of magnitude smaller than that exerted on atoms in the outermost atomic plane. This comparison reflects the fact that, compared to an atom in the outermost substrate layer, a substrate atom in the second layer sits in a scattering environment that more closely resembles an atom deep inside the bulk crystal (for which the wind force vanishes). The rapid decay of the wind force into the bulk suggests that the substrate forces arising from carrier scattering at the Ag(111) surface are localized within the first one or two atomic planes of the substrate.

Assuming that τ is equal to the bulk relaxation time [8260 a.u. at 77 K, 1652 a.u. at 273 K (Ref. 31)] these calculated wind forces correspond to effective valences, in the outermost layer of Ag(111), of $(Z_w^{xx}, Z_w^{yy}) = (-50.4, -49.6)$ at 77 K and $(Z_w^{xx}, Z_w^{yy}) = (-10.1, -9.9)$ at 273 K. We note that, in general, the relaxation time at the surface may be different to that of the bulk. Therefore, in the absence of accurate calculations of τ for carrier scattering of the surfaces of metals, we must regard these values as only estimates of the true wind valence of the adatom.

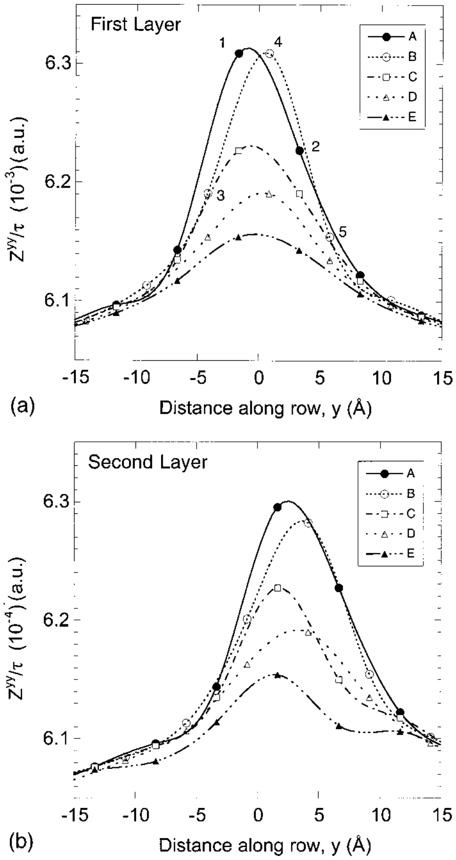

FIG. 2. The effective wind valence Z^{yy} of atoms within the outermost two atomic layers of the Ag(111) substrate when an Ag adatom is adsorbed at the fcc hollow site: (a) Outermost layer, (b) second layer. The wind valence of each atom is normalized to the relaxation time, Z_w^{yy}/τ, and is plotted as a function of the *y* coordinate of the atom within each row, measured relative to the fcc hollow site (at $y=0$). Each curve corresponds to one of the the atomic rows, (*A*, *B*, *C*,...) identified in Fig. 1 and the line is a guide to the eye only. For clarity, the data points corresponding to substrate atoms labeled in Fig. 1 are numbered.

Next we computed the wind force exerted upon an Ag adatom placed in the three high-symmetry adsorption sites shown in Fig. 1. The magnitude of the calculated wind force, parallel to the applied field along the [10] direction, was $Z_w^{xx}/\tau = -1.02\times10^{-2}$, -1.02×10^{-2}, and -1.24×10^{-2} a.u. for the fcc, hcp, or twofold bridge sites, respectively. These valences are almost identical to those obtained when the field is applied parallel to the $[\bar{1}2]$ direction: $Z_w^{yy}/\tau = -1.00\times10^{-2}$, -1.00×10^{-2}, and -1.23×10^{-2} a.u., respectively. We note that the wind forces experienced by the adatom are a factor of 1.7–2.0 larger than the forces exerted on an atom in the top layer of the clean Ag(111) surface. Again, this is a reflection of the fact that the substrate atom sits in a scattering environment that more closely resembles an atom deep inside the bulk crystal. Assuming, again, that τ is equal to the relaxation time in bulk Ag, the effective valences of the Ag adatom at 273 K are $(Z_w^{xx}, Z_w^{yy}) = (-16.8, -16.5)$ for the fcc site, $(-16.8, -16.5)$ for the hcp site, and $(-20.5, -20.3)$ for the bridge site.

In Fig. 2 we plot the magnitude of the calculated wind valences, Z_w^{yy}, of the substrate atoms in the vicinity of an Ag

TABLE I. The calculated wind valences for adsorption of an Ag adatom at the three high-symmetry adsorption sites of Ag (111). The wind valence Z_w/τ is normalized to the relaxation time τ and is expressed in atomic units (where 1 a.u. = 0.024 18 fs. The table contains the diagonal components of the calculated wind valence tensor of the adatom. These quantities describe the component of the wind force parallel to the electric field when it is applied along the $[10](Z_w^{xx})$ and $[\bar{1}2](Z^{yy})$ directions (see Fig. 1). ΔZ_w is the sum of the change in the effective wind valences of Ag atoms, within each of the substrate layers, that is induced by the presence of the adatom. Also given is the percentage of the momentum transferred from the carriers that goes to the adatom and to the substrate atoms.

Wind valence ($\times 10^{-2}$) a.u.	fcc site	hcp site	Bridge site	No adatom
Adatom Z_w^{xx}/τ	-1.02	-1.02	-1.24	
Substrate layer 1$\Delta Z_w^{xx}/\tau$	-1.80	-1.80	-1.63	-0.61
Substrate layer 2$\Delta Z_w^{xx}/\tau$	-0.39	-0.39	-0.26	-0.06
Total $\Delta Z_w^{xx}/\tau$	-2.19	-2.19	-1.89	-0.67
Adatom:substrate (%)	32:67	32:67	40:60	0:100
Adatom, Z_w^{yy}/τ	-1.00	-1.00	-1.23	
Substrate layer 1$\Delta Z_w^{yy}/\tau$	-1.98	-1.97	-1.87	-0.60
Substrate layer 2$\Delta Z_w^{yy}/\tau$	-0.43	-0.43	-0.30	-0.06
Total $\Delta Z_w^{xx}/\tau$	-2.41	-2.40	-2.17	-0.66
Adatom:substrate (%)	29:71	29:71	36:64	0:100

adatom adsorbed onto the threefold fcc hollow site. The electric field is parallel to the $[\bar{1}2]$ direction, and the components of the wind force, parallel to the field, acting upon each of the atoms within the outermost and second atomic layers are shown. The results obtained for the field parallel to the [10] direction (not shown) are qualitatively similar to those shown in this figure. From Fig. 2 it is apparent that the carrier scattering by the adatom alters the magnitude of the wind force felt by substrate atoms near the adsorption site. Although the *change* in the force exerted upon each the substrate atoms is relatively small compared the magnitude of the force itself, the change in the *total* force (summed over all substrate atoms around the adsorption site) is significant. Our results for the summed forces are summarized in Table I where we have defined

$$\Delta Z_w^{ij} \equiv \sum_k \delta(Z_w^k)^{ij}. \tag{5}$$

Here the sum is taken over all substrate atoms in the first and second layers. We find that $(\Delta Z_w^{xx}/\tau, \Delta Z_w^{yy}/\tau) = (2.19\times 10^{-2}, 2.41\times 10^{-2})$ a.u., when the adatom is in the fcc site, $(2.18\times 10^{-2}, 2.40\times 10^{-2})$ a.u. when the adatom is in the hcp site, and $(1.89\times 10^{-2}, 2.16\times 10^{-2})$ a.u., when the adatom is placed in the twofold bridge sites.

By comparing the wind valence of the adatom, Z_w^{ij}, to the change in total the wind valence summed over the substrate atoms, ΔZ_w^{ij}, we can determine how the momentum transferred from the carriers is partitioned between the adatom and the substrate (see Table I). For example, for adatom adsorption into the fcc hollow site, the calculated wind valences of the adatom are $Z_w^{xx}/\tau = -1.02\times 10^{-2}$ a.u. and $Z_w^{yy}/\tau = -1.00\times 10^{-2}$ a.u. The corresponding change in the net calculated wind valence of the substrate atoms is $(\Delta Z_w^{xx}/\tau, \Delta Z_w^{yy}/\tau) = (2.19\times 10^{-2}, 2.41\times 10^{-2})$ a.u. Therefore, when the adatom is adsorbed onto the surface, only approximately 32% of the additional momentum transferred from the carriers goes to producing the wind force actually felt by the adatom. The remaining ~68% of net momentum transfer from the carriers is exchanged with the substrate atoms. A similar analysis of our results for the adatom adsorption into hcp and bridge sites is given in Table I. These results indicate that the wind force felt by the adatom is responsible for less than one-half of the additional momentum transferred between the carriers and the surface. Therefore, for Ag on Ag(111), only part of the increase in the surface resistivity that is induced by the adatom can be associated directly with the wind force felt by the adatom. Consequently, the simple relationship between the surface induced resistivity and the adatom wind force, expressed in Eq. (2), is of limited validity when applied to this system. Nevertheless, Eq. (2) can be used to estimate the surface induced resistivity if it is rewritten in terms of the total force exerted on the surface.[20] Then, for a metallic film with thickness l_f, the initial rate of increase of the surface resistivity with the areal density of adatoms is

$$l_f \frac{\partial \rho_s}{\partial \eta_a}\bigg|_{n_a \to 0} = -\frac{1}{e\eta \mathbf{J}}\left(\mathbf{F}_w^a + \sum_j \delta \mathbf{F}_w^j\right) = -\frac{m^*}{e^2\eta^2}\frac{(Z_w^a + \Delta Z_w^s)}{\tau}. \tag{6}$$

Substituting into Eq. (6) the calculated wind valences for adatom adsorption into the fcc hollow site and using the bulk carrier density, $\eta = 0.0585$ Å^{-3},[32] we find that the initial rate of increase of the $[l_f \rho_s]$ with η_a is equal to 1440 $\mu\Omega$ cm Å^3 for ρ_s^{xx} and 1530 $\mu\Omega$ cm Å^3 for ρ_s^{yy}. These estimates can be compared with the value derived from resistivity measurements for Ag adsorption on Ag thin films: 2170 ± 170 $\mu\Omega$ cm Å^3.[2,8] Our underestimate of the change in the surface-induced resistivity originates from our use of the bulk carrier density in the evaluation of Eq. (6); the effective carrier density in the vicinity of the adatom should be smaller than the bulk value, reflecting the reduction of coordination in the surface region. We note that if Eq. (6) is evaluated neglecting the momentum transfer to the substrate atoms ($\Delta Z_w^s = 0$), then the the initial rate of increase of the $[l_f \rho_s]$ with η_a is found to be much smaller: 458 $\mu\Omega\,\mathrm{cm}\,\text{Å}^3$ for ρ_s^{xx}. This value is more than a factor of 4 smaller than the measured value, representing a significant level of quantitative disagreement. This comparison emphasizes the importance of the momentum transfer to the substrate in determining the actual surface resistivity induced by an Ag atom on Ag(111).

In summary, we have used a layer Korringa-Kohn-Rostoker calculation to study the relationship between the electromigration wind force and the surface resistivity induced by an isolated Ag adatom on Ag(111). By computing the wind forces felt by both the adatom and atoms within the substrate, we have shown that the presence of the adatom significantly alters the magnitude of the wind force exerted on substrate atoms that are close to the adsorption site. We find that only approximately 30%–40% of the momentum transferred from the carriers impinging upon the surface goes to producing the wind force on the adatom. This partitioning of the momentum transfer among the adatom and the substrate atoms significantly alters the usual relationship between F_w and $\Delta\rho_s$ that was derived using jellium models of the substrate. We have also shown that reasonable quantitative agreement with the measured change in the surface resistivity of Ag/Ag(111) can only be obtained if the carrier scattering between the substrate atoms and adatom is considered explicitly.

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