The Electromigration Force in Metallic Bulk

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Abstract. The voltage induced driving force on a migrating atom in a metallic system is discussed in the perspective of the Hellmann-Feynman force concept, local screening concepts and the linear-response approach. Since the force operator is well defined in quantum mechanics it appears to be only confusing to refer to the Hellmann-Feynman theorem in the context of electromigration. Local screening concepts are shown to be mainly of historical value. The physics involved is completely represented in ab initio local density treatments of dilute alloys and the implementation does not require additional precautions about screening, being typical for jellium treatments. The linear-response approach is shown to be a reliable guide in deciding about the two contributions to the driving force, the direct force and the wind force.

Results are given for the wind valence for electromigration in a number of FCC and BCC metals, calculated using an ab initio KKR-Green’s function description of a dilute alloy.

INTRODUCTION

Electromigration in a metal, being the drift of atoms under the influence of an electric field, is interesting from different points of view [1]. From the theoretical side a question arose about the screening of the charge of the migrating particle. This question was the subject of a long-standing controversy, which has been clarified to a large extent only recently [2, 3]. On the technological side the problem of the failure of integrated circuits, the so-called aluminum catastrophe, has attracted attention up to now. This problem has mainly been approached empirically, which has led to the observation that the addition of copper impurities slows down the development of voids. For a long time this electromigration induced failure was attributed to the high diffusion rate along grain boundaries. Recently, ongoing miniaturization has led to interconnects with a bamboo structure [4], in which interface and bulk diffusion are becoming more and more important [5].

In any attempt to describe the process of electromigration one uses the conventional decomposition of the driving force $F$ in an electrostatic direct
force, and a wind force attributed to momentum transfer of the current carrying electrons to the migrating atom,

\[ \mathbf{F} = \mathbf{F}_{\text{direct}} + \mathbf{F}_{\text{wind}} = (Z_{\text{direct}} + Z_{\text{wind}}) e \mathbf{E} = Z^* e \mathbf{E}. \]  

(1)

The forces are proportional to corresponding valences and the applied electric field \( \mathbf{E} \). The effective valence \( Z^* \) is the measurable quantity. A basic task of the theory of electromigration is to provide with a microscopically correct expression for the driving force.

In a history of over thirty years this task has not been achieved completely yet. This is certainly due to the complexity of the phenomenon of electromigration. Although the force is a local quantity, the presence of a current density requires the treatment of a macroscopically large system. Semiclassical treatments, along with fully quantum-mechanical ones, were supplemented by momentum-balance considerations, the latter being obscured by a treacherous interpretation dependence. Also the force according to the Hellmann-Feynman theorem was considered [6, 7, 8]. For a review of the various approaches, including a clearly structured account of a new linear-response result for the driving force, see Ref. [3].

Still, we think that due to new developments, both on the fundamental level of deriving a reliable expression for the driving force and on the practical level of doing actual calculations of the wind valence in real metals, things have become much clearer than fifteen years ago. We will illustrate that first by discussing the Hellmann-Feynman theorem in relation to the driving force. After that the merit of local concepts such as the residual-resistivity dipole will be evaluated, using linear-response theory and results from \textit{ab initio} calculations. Finally, results will be presented for the wind valence in FCC and BCC metals.

**HELLMANN-FEYNMAN THEOREM AND DRIVING FORCE**

An appealing expression for the driving force on an atom at position \( \mathbf{R}_p \),

\[ \mathbf{F}_p = Z_{\text{direct}} e \mathbf{E} - \int \delta n(r) \nabla_{\mathbf{R}_p} v_p d^3r, \]  

(2)

is found in many papers [9, 10]. Since \( \delta n(r) \) is the deviation of the local electron density from the equilibrium density, being linear in the electric field, the second term is viewed as an obvious form for the wind force, \( - \nabla_{\mathbf{R}_p} v_p \) being the operator for the force on the atom. This equation was already described by Bosvieux and Friedel [11], but in their formalism \( Z_{\text{direct}} \) turned out to be zero.
for an interstitial atom. The latter fact gave rise to the controversy mentioned above, to which we will return later on. Eq. (2) is also reminiscent of the force expression following from Feynman’s theorem, dating back to the early days of quantum chemistry calculations [8]. Here we want to add to the discussion started by Sorbello and Dasgupta [6] about the relationship between the two.

Feynman derived the equality

$$\nabla_{\lambda} \mathcal{E}(\lambda) = \langle \psi_{\lambda} | \nabla_{\lambda} H(\lambda) | \psi_{\lambda} \rangle,$$

(3)

in order to facilitate quantum-chemistry calculations of the equilibrium configuration of atoms in a molecule. One was used to calculate the ground state energy $$E(\lambda) = \langle \psi_{\lambda} | H(\lambda) | \psi_{\lambda} \rangle$$ as a function of a parameter $$\lambda$$, for example the $$x$$ component of the position of an atom. By varying the value of $$\lambda$$ and repeating the calculation for the $$y$$ and $$z$$ components, one determined the direction of evolution toward an equilibrium configuration. In this perspective Eq. (3) is very helpful in calculating the force at a position corresponding to a value of $$\lambda$$, because one can restrict oneself to the calculation of one matrix element for that value of $$\lambda$$, the matrix element at the right-hand side of this equation.

Now consider a system of a free molecule under the influence of a uniform electric field. In addition to the potentials $$V_j$$ of the nuclei at positions $$R_j$$, the Hamiltonian contains a term $$-\sum_j Z_j e R_j E$$ and a similar term for the electrons interacting with the field. Applying Eq. (3) for $$\lambda = R_p$$, one finds for the so-called Hellmann-Feynman force

$$F_{HF}^p = -\nabla_{R_p} \mathcal{E}(R_p) = Z_p e E - \langle \psi_{R_p} | \nabla_{R_p} V_p | \psi_{R_p} \rangle + \sum_{j(\neq p)} F_{pj}.$$

(4)

The third term corresponds to the force on the nucleus at the position $$R_p$$ due to repulsion by the other nuclei. Since $$V_p = \sum_i v_0^p (r_i - R_p)$$ is a sum over all electrons, at positions $$r_i$$, of the nuclear potential $$v_0^p$$, the many-body matrix element in Eq. (3) can be written as a one-body integral over the electron density, by which this equation becomes [6]

$$F_{HF}^p = Z_p e E - \int n(r, \{R_j\}, E) \nabla_{R_p} v_0^p d^3r + \sum_{j(\neq p)} F_{pj}.$$

(5)

For a molecule with the nuclei at equilibrium positions, the second term with $$E = 0$$ cancels the third one. Then the force $$\delta F_{HF}^p$$, purely induced by the applied field, can be written as

$$\delta F_{HF}^p = Z_p e E - \int \delta n(r, \{R_j\}, E) \nabla_{R_p} v_0^p d^3r,$$

(6)

which is proportional to the field $$E$$ and is most similar to Eq. (3). Sorbello et al. [6] evaluated Eq. (3) for an isolated one-electron atom and showed
explicitly that the force cancels, as it should. The force (8) remains finite for a nucleus in a molecule. Only the total force, the sum $\sum_p \delta F_p$, cancels.

The Hellmann-Feynman theorem was derived for a finite system such as a molecule. Although electromigration occurs in a current carrying solid, due to the similarity of Eqs. (2) and (8) one might wonder whether still there is a relation between the two. In order to understand why the final answer is negative, one has to analyze the ingredients of the theorem (3). First, the system is bound to be finite because the total energy $\mathcal{E}(\lambda)$ is the starting point. Secondly, and we think more importantly, a single ground state $\psi_\lambda$ is supposed to be available or calculable.

Since most of the theories for solids use a finite volume and periodic boundary conditions, the first limitation is not serious. That is why one still refers to it [12] in doing electrostatics calculations on lattice distortion around an impurity. In taking the thermodynamic limit, \textit{i.e.} going to infinite volume and keeping the density constant, the volume factors drop out and the summations turn into integrals, which, ironically, in present days are evaluated numerically as summations. In electrostatics calculations one effectively operates at absolute zero temperature, the Fermi surface is sharp and one can work with the concept of a ground state. In electromigration, however, and in dealing with any transport property, this is obviously not the case. One has to work at a finite temperature. The system cannot be described with a single wave function $\psi_{\mathbf{R}_p}$. A macrocanonical ensemble of states has to be used. One has to turn to the means developed in non-equilibrium quantum statistical mechanics. To that end a Kubo-formula like linear-response expression for the driving force was proposed by Kumar and Sorbello [13].

It seems legitimate to ask what nowadays is still the message of the Hellmann-Feynman theorem (3), particularly in calculating local forces in systems. For that purpose the equality (3) seems to be a trivial one. We consider it as a possible answer, that in the early days of quantum mechanics a force operator was more or less suspect, reminding too much of newtonian classical mechanics. A Hamiltonian and the energy were considered as reliable objects. Nowadays we know that the force operator is a reliable object as well, and Eq. (3) just confirms that fact.

Taking things together, referring to Eq. (3) in electrostatics calculations is not necessary, because one actually calculates the expectation value of the force operator. Authors still continue to do so, but it merely serves as a label that physicists recognize. Referring to the Hellmann-Feynman theorem in electromigration theory is even confusing. One has to concentrate on the evaluation of the force operator in a statistical ensemble, while the Hellmann-Feynman theorem deals with a single ground state only, and does not give a clue how to go beyond that.

We conclude this section by a discussion of the linear-response expression
for the driving force, which can be derived from the quantum-statistical expectation value of the force operator, directly coming from the commutator of the momentum operator $P_p$ with the total Hamiltonian,

$$F_p = \text{Tr}\{\rho \frac{dP_p}{dt}\} = Z_p eE - \text{Tr}\{\rho \nabla_{R_p} V_p\}. \quad (7)$$

The many-body linear-response form can be simplified to the form $[14]$

$$F_p = Z_p eE - ie \lim_{\alpha \to 0} \int_0^\infty dte^{-\alpha t} \text{tr}\{n(h)[f_p(t), \mathbf{r} \cdot \mathbf{E}]\}, \quad (8)$$

for any system with an unperturbed Hamiltonian $H$ that can be written as a sum of single-electron Hamiltonians

$$H = \sum_i h^i. \quad (9)$$

The latter property holds for the electron-impurity model system described in the local density approximation, its most simple realization being the impurity-in-a-jellium model. In such a model system electron-phonon interaction is not accounted for, but it is good to realize, that almost all evaluations of Eq. (8) or its many-body form pertain merely to the electron-impurity model system. In Eq. (8) the time dependence of the force operator $f_p = -\nabla_{R_p} v_p$ is given by

$$f_p(t) = e^{iht}f_pe^{-iht}, \quad (10)$$

while $n(h)$ is the Fermi-Dirac distribution in operator form

$$n(h) = \frac{1}{e^{-\beta(h-\epsilon_F)} + 1}, \quad (11)$$

$\epsilon_F$ being the Fermi energy and $\beta^{-1} = k_B T$. Comparing Eq. (8) with Eq. (4), one is inclined to identify the second term in Eq. (8) as the wind force. In evaluating the trace operator in the linear-response expression, Sham $[15]$ already found that this identification holds only partially. In addition to the real wind force he found a screening contribution, to be combined with the unscreened first term in Eq. (8).

Sham evaluated a many-body expression, but his result can be read quite simply from Eq. (8), which has been proven to be equivalent to Sham’s expression $[14]$. The real wind force follows from the second term in this equation after the replacement of the one-electron system Hamiltonian,

$$h = h_0 + \sum_j v_j, \quad (12)$$

in the statistical factor $n(h)$, by its unperturbed part $h_0$, $v_j$ being the electron-impurity potential for the impurity at the position $R_j$. Sham proved this to
lowest order in the electron-impurity potential, and it appears to hold to all orders, which are generated by the time dependent factors around the force operator \([16]\). The screening contribution comes from what is left, namely a term with \(n(h) - n(h_0)\) instead of \(n(h)\). To lowest order in the electron-impurity potential Sham found a negligible screening contribution. Recently \([14]\) his result has been confirmed, but in addition it was shown to be possible to evaluate the expression to all orders. That analysis leads to a complete cancellation of the direct force. Some objections were raised \([17, 18]\), but it was not difficult to unravel them \([19, 20]\). Although the proof is valid only for the electron-impurity system, it settles an important point in the controversy. Sham’s result has been used again and again in arguing in favour of an unscreened direct force \([10, 21]\). The argument was, that a lowest order result, being quadratic in the potential, and therefore quadratic in \(Z_p\), logically excludes a complete cancellation of the linear unscreened force.

Unfortunately, experiments on hydrogen in V, Nb and Ta, set up to decide in this matter, turned out to be not conclusive \([22]\). Although complete screening could be excluded, for hydrogen in Nb the fitting procedure resulted in the rather small direct valence value of 0.44. An attempt to account for electron-phonon interaction points in the direction of a reduced screening on increasing the temperature \([2, 23]\). Since this attempt is not an exact result, the question about the screening of the direct force cannot be considered as completely settled yet.

Local screening-field approaches will be discussed in the following section.

**LOCAL CONCEPTS AND DRIVING FORCE**

Parallel to the formulation of the driving force according to a Kubo formula approach \([13, 14, 15]\), a local screening field approach has been applied, inspired by Landauer \([24, 25, 26]\). Illustrative examples of recent work are the treatment of electromigration in mesoscopic systems by Sorbello \([10]\) and a direct force calculation by Ishida \([27]\). Landauer’s concepts leading to the wind and direct forces are the residual resistivity dipole \([25, 28]\) and carrier density modulations \([26, 27]\) respectively. Although it is accepted that these concepts cover an aspect of the physical reality of electronic behaviour in the neighbourhood of an impurity in a metal \([28]\), it is admitted that they neither have led to new answers for the residual or impurity resistivity \([28, 29]\), nor have contributed to the resolution of the controversy about the driving force in electromigration. In the present section we want to comment on recent work \([10, 27, 30]\), keeping in mind the result of complete screening of the direct force on an impurity in a jellium, obtained using a Kubo-formula approach \([14]\).

In dealing with electromigration in mesoscopic systems, Sorbello \([10]\) finds
an expression for the wind force equivalent to the second term in Eq. (2) and completely in agreement with the original Bosvieux-Friedel expression and later generalizations of it used in metallic systems. His expression for the direct force contains two terms, an unscreened term and a term accounting for screening, which composition is in agreement with the Kubo-formula analyses discussed above. His method is based on treating local transport fields at and around an impurity immersed in a ballistic mesoscopic environment, being essentially a jellium environment. Electron-phonon interaction is negligible, because in his model systems the inelastic electron mean-free-path exceeds the system size. Screening is dealt with according to well established jellium rules.

For two of the three model systems considered he finds a vanishing direct force. In evaluating the direct force in his third model system, an impurity in the vicinity of a point contact, he does not find complete screening. It is most interesting to observe, that in obtaining this latter result an argument was used derived from a consensus interpretation of incomplete linear-response treatments, the presently available complete treatment not being published yet at that time. That may explain the struggle of the author with what he calls a paradox, and his inclination to distrust the Kubo approach.

Ishida studies the simple system of one impurity in a jellium, and finds a small screening only. This contradicts the exact Kubo-formula result and is not in agreement with Sorbello’s findings either. An objection as that in the Kubo-formula approach the screening is not accounted for self-consistently, is not valid. By starting from the complete Hamiltonian and evaluating the exact formal expression, all dynamics in the system is accounted for. The cause of Ishida’s different result was uncovered in a discussion with the author. Ishida uses an ac field in order to avoid infinities in his wind force. However, the infinitesimally small \( a \) as it occurs in Eq. (8), which comes from the adiabatic switching-on of the electric field and plays the role of the inverse relaxation time if no dissipative scattering is present, was not treated with sufficient care. Although Ishida is speaking about a small frequency \( \omega \), all his results are in the large frequency domain, because \( \omega/a \) is always much larger than unity, irrespective how small \( \omega \) is. In the \( \omega \to 0 \) limit, so in the true dc limit, his formalism also leads to complete screening.

Kandel and Kaxiras calculated the direct force on a Si atom on top of a Si surface. In this semiconductor problem the wind force turns out to be negligible. Through a self-consistent calculation they find a very small direct valence of 0.05, but it is significantly different from zero. In a semiconductor environment, with dangling bonds, a complete screening is not expected a priori, but the actually calculated direct valence is very small indeed.

Taking everything together, more and more results are pointing into the
direction of a screened direct force for an impurity in an electron gas. Still, it remains true that this point has not completely been settled yet, even apart from a possible reduced screening due to electron-phonon interaction [2, 23].

Now let us turn to the wind force, which is equally present in all treatments. In discussing the meaning of the residual resistivity dipole (RRD), it is useful to introduce first the well-established expression used in practical calculations for metallic systems [3, 10, 36, 37].

\[
F_{\text{wind}} = \sum_{\mathbf{k}} \delta f(\mathbf{k}) \langle \Psi_{\mathbf{k}} | - \nabla_{\mathbf{R}_p} v_p | \Psi_{\mathbf{k}} \rangle.
\] (13)

The deviation \(\delta f(\mathbf{k})\) from the Fermi-Dirac distribution, here denoted by \(f_0(\epsilon_{\mathbf{k}})\) instead of by \(n(\epsilon_{\mathbf{k}})\) (see Eq. [11]),

\[
\delta f(\mathbf{k}) = e \tau \mathbf{E} \cdot \mathbf{v}_k \frac{d}{d\epsilon_k} f_0(\epsilon_{\mathbf{k}})
\] (14)

is a result of the applied electric field \(\mathbf{E}\). The sum over the states, labeled by \(\mathbf{k}\), can be written as \(\delta n(\mathbf{r})\), after which one recognizes the second term in the basic expression [2]. So, the wind force is proportional to the mean free transport time \(\tau\) of electrons and therefore inversely proportional to the resistivity of the sample. The electronic structure is represented by the wave function \(\Psi_{\mathbf{k}}\) and the scattering is taken care of by the potential \(v_p\) of the migrating atom.

In applications to dilute alloys [37] the wave function \(\Psi_{\mathbf{k}}\) is calculated using multiple-scattering theory. The electronic structure of the unperturbed metallic host is calculated by the Korringa-Kohn-Rostoker (KKR) method [38, 39]. Since \(\Psi_{\mathbf{k}}\) is the exact local wave function the electronic structure of the electromigration defect has to be calculated, consisting of the migrating atom, its near surroundings, possibly being affected by charge transfer and lattice distortion, and, in the case of substitutional electromigration, a neighbouring vacancy. For that purpose an advanced application of multiple-scattering theory is used, called KKR Green’s function theory [36, 37, 40]. It may be useful to remark, that the wind force given by Eq. (13) depends on the position \(\mathbf{R}_p\) of the migrating atom along its jump path. This holds irrespective whether one considers migration of an interstitial or a substitutional atom, the latter requiring a neighbouring vacancy. The actually measured force \(\mathbf{F}\) is calculated from the work done by the position dependent force \(\mathbf{F}_p\) along the path, divided by the path length, and averaged over the possible orientations of the path with respect to the \(\mathbf{E}\) direction. In the following section \textit{ab initio} results will we given for \(Z_{\text{wind}}\) calculated that way, for a number of FCC and BCC metals.

Here we want to give a special result related to the RRD. In Fig. [9] the wind force is shown as it acts on vanadium atoms around a vacancy in V. Position 1 is the initial position in an actual migration jump. One sees that,
Figure 1: Wind force on a V atom next to a vacancy, indicated by a dotted circle, for different orientations of the migration path with respect to the electric field $E$. For position 1 the field lies along the migration path. For positions 3 and 4 it points perpendicular to it.

going from position 1, via the perpendicular positions 3 and 4, to position 2, so looking around half a circle, the direction of the force turns over $360^\circ$. Interpreting the force direction as showing the local current direction, the vacancy apparently induces a back flow. Such an effect is covered by the concept of the RRD. This can be seen as follows.

In discussing the RRD always an impurity in a free-electron medium, or, equivalently, a jellium is considered, while the dissipative property of the medium is represented by a transport relaxation time $[28, 29]$. Following Sorbello $[28]$ in a slightly generalized form, the wave function $\Psi_k$ can be written as

$$\Psi_k(r) = \frac{4\pi}{\sqrt{\Omega}} \sum_{\ell m} i^\ell Y_{\ell m}(\hat{k}) R_{\ell}(r) Y_{\ell m}(\hat{r}),$$  \hspace{1cm} (15)

$\Omega$ being the volume of the system, and the radial wave function having the following asymptotic behaviour

$$R_{\ell}(r) = j_\ell(kr) + i\sin\delta_\ell e^{i\delta_\ell} h_{\ell}^+(kr).$$  \hspace{1cm} (16)

Here $j_\ell$ and $h_{\ell}^+$ are the spherical Bessel and Hankel functions respectively, and $\delta_\ell$ are the phase shifts of the scattering potential. It is clear that the Bessel function part of $\Psi_k(r)$ sums precisely up to the normalized plane wave $e^{ikr}/\sqrt{\Omega}$. Using that the derivative of the Fermi-Dirac distribution $f_0(\epsilon_k)$ with respect to the energy $\epsilon_k$ effectively is equal to $-\delta(\epsilon_k - \epsilon_F)$, and restricting oneself to $s$ scatterers, one finds, that $\delta n(r)$, according the Eqs. (2) and (13) given by $\sum_k \delta f(k)|\Psi_k(r)|^2$, becomes equal to

$$\delta n(r) = A E \cdot \hat{r} \sin\delta j_1(kr) \left[ \cos\delta j_0(kr) - \sin\delta n_0(kr) \right] \equiv A E \cdot r g(r),$$  \hspace{1cm} (17)
in which $A$ is a positive constant equal to $2e\tau k_F^2/\pi^2$. Only the $\ell = 0$ phase shift, denoted by $\delta$, is left. This expression clearly has a dipolar form. Sorbello [28] even distinguishes a Bosvieux-Friedel dipole, given by the first term, and a RRD dipole proportional to $\sin^2 \delta$.

Now the wind force can be calculated for a configuration as in Fig. 1. Modeling the vacancy by a strong $s$ scatterer, and a surrounding atom by a weak potential, centered at $R$, the following integral

$$F_{\text{wind}} = -A \int E \cdot r g(r) \nabla_R v(r - R) d^3r = -A \nabla_R \int E \cdot r g(r) v(r - R) d^3r \quad (18)$$

has to be evaluated. A most simple, but illustrative result is obtained for an attractive delta function potential $v(r - R) = -C \delta(r - R)$ with a small positive constant $C$. One finds

$$F_{\text{wind}} = AC[E g(R) + (E \cdot \hat{R}) R g'(R)]. \quad (19)$$

This force has a behaviour which is similar to what is depicted in Fig. 1. The first term points along the field and is proportional to $g(R)$. The second term, being proportional to $R g'(R)$, points along $R$, but its direction changes sign, and so turns over $180^\circ$, when $R$ is perpendicular to $E$. So its direction turns over $360^\circ$ while $R$ turns over $180^\circ$. The precise behaviour depends on the ratio $R \frac{d}{dR} \ln g(R)$. A typical value of this ratio is $-2$, by which the second term dominates at the positions 1 and 2. Due to its negative value the forces according to Eq. (19) have a direction opposite to the forces in Fig. 1. This is consistent with a jellium treatment, which can give a negative $Z_{\text{wind}}$ only.

Although existing evaluations of the RRD are given for an impurity in a jellium only, Fig. 1 shows that a RRD is also present in a real solid. Nevertheless, in doing actual calculations of the wind force the concept of a RRD does not enter at all. One might wonder what is the reason. As it has already been indicated earlier [16, 28], the RRD is accounted for automatically in a complete multiple-scattering calculation. The concept does not enter the formulation. It can be considered as a manifestation of Landauer’s physical intuition that he pointed at such local effects, higher than to second order in the potential, before one devised the means to make them explicit in a complete scattering theory [24]. Further, the concept is helpful in resolving a paradox in the calculation of the impurity resistivity using statistical mechanics. In the latter treatment only elastic scattering enters, and dissipation cannot be understood. The RRD makes it clear that a local field is building up. But in practice the concept is not of much help, and it is mainly of historical value. As quoted above [25, 29], it has never led to new answers in treating transport properties.
Ab Initio RESULTS FOR THE WIND FORCE

*Ab initio* results for the wind valence in a number of FCC and BCC metals are given in Table 1. The majority of the results presented apply to self-electromigration. For impurity migration in a metal M the system is indicated as M(I). The calculation for a HCP metal such as Zr was carried out by using the corresponding FCC structure. Note, that Zr occurs in the BCC column as well. This is done because Zr undergoes a structural phase transition from HCP to BCC on approaching the melting temperature $T_m$. All $Z_{\text{wind}}$ values are at 0.9 $T_m$. If one is interested in the value at another temperature $T$, one just has to look up the resistivity values at 0.9 $T_m$ and $T$, and to substitute them in the following equality

$$Z_{\text{wind}}(T) = Z_{\text{wind}}(0.9 T_m) \rho(0.9 T_m)/\rho(T).$$

The agreement with the limited experimental values [41, 42] appears to be quite reasonable, particularly considering that no self-consistent potentials
were available. Further we want to draw the attention to three typical features. First one sees that both positive and negative wind valences are found. This is a result of the detailed electronic structure of the system, and it could never come from a jellium calculation, leading always to a negative wind valence. Secondly, it is interesting to observe, that two impurities in the same metal, e.g. Zr and Tc in Nb, have different signs of the wind valence. At first sight this is counterintuitive, if one considers the current flow in the host metal as being decisive for the sign of the wind valence. However, in the formalism all scattering effects are taken into account. A typical multiple-scattering effect of an impurity in a metal is the back-scattering, which can be much different for different impurities. Finally, $Z_{\text{wind}}$ appears to be rather small for quite a number of metals. This means, that a measurement of the effective valence $Z^*$ will be valuable in the determination of the direct valence.

**CONCLUSIONS AND PERSPECTIVES**

In discussing the Hellmann-Feynman theorem in relation to the driving force in electromigration, it is made clear that the latter requires the tools developed in statistical mechanics, to which the theorem does not give a clue. The theorem can be considered as being only of historical value, in providing confidence in the force operator as a proper quantum mechanical entity.

A reliable expression for the wind force is available, being applicable in real systems, such as metals and dilute alloys. Strong evidence is available for cancellation of the direct force on an impurity embedded in an electron gas, so that only the wind force is left, although some results do not confirm this yet. The influence of electron-phonon interaction on this cancellation is still not entirely clear.

Local concepts are illustrated to cover real entities, but in the actual theory applied in practical calculations they do not enter. That is why these concepts never have led to new answers in dealing with transport properties. Reality is completely covered by a standard calculation accounting for all scattering effects. The most powerful method available at present is the KKR-Green function theory. The *ab initio* obtained wind forces in a number of FCC and BCC metals can be of practical value. They can be used also in deciding about the direct force, because in several systems the wind force turns out to be very small.

Up to now results are available for bulk electromigration only. For substitutional electromigration this implies a configuration of a migrating atom exchanging position with a neighboring vacancy. We want to stipulate that the formalism allows for treatment of much more flexible configurations, which could simulate both surface electromigration and migration along a grain.
boundary. The complete electromigration defect accounted for consists of 20 and 16 scattering centers in the FCC and BCC structures resp. This defect consists of the migrating atom, including its initial and final position, and all neighboring perturbed metallic atoms around these two positions. By omitting more and more atoms in the defect one can gradually generate a void. It is well possible to calculate the wind force on an atom moving in such a void along the inner metallic surface. Such a configuration would simulate surface electromigration. Other configurations can be designed to simulate a grain boundary. It is most promising to look to such configurations in the near future.

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