

a Yukawa-potential type expression. The Born-Mayer contribution is a simple exponentially-decaying function of the core-core separation, motivated by the radial decay of electron wavefunctions for the closed shells. The effective interatomic potential reads as

$$V(r) = A \frac{\exp^{-q_{\text{TF}}(r-2a_0)}}{r-2a_0} + B e^{-C(r-\bar{\sigma})} \quad (1)$$

where

$$A = Z_{\text{ion}}^2 e^2 \cosh^2(q_{\text{TF}} R_{\text{core}}) \quad (2)$$

is the Ashcroft factor [20], with  $R_{\text{core}}$  being a typical value for the atom-specific core radius and  $Z_{\text{ion}}$  the effective ionic charge number. Furthermore,  $a_0$  is the Bohr radius and  $\bar{\sigma}$  is the average ionic core diameter of the alloy, which corresponds to the average size of the ionized atoms constituting the alloy. The average ionic core diameter is obtained by averaging the respective ionic core diameter of the constituents with their contributing weights given by their volume ratios in the alloy. The values for the ionic core diameters of the atoms constituting the alloys are taken from Ref. [21].

The quantities  $A$  and  $B$  set the energy scales for the repulsive interaction from the Ashcroft and Born-Mayer term, respectively. The parameter  $q_{\text{TF}}$  is the inverse of the Thomas-Fermi screening length given by Thomas-Fermi theory, and its value is known for different types of alloys [22]. We choose a representative value for  $q_{\text{TF}}$  as  $1.7 \text{ \AA}^{-1}$  according to the values reported in Ref. [22]. The ionic core diameter  $\bar{\sigma}$  is obtained by a weighted average of the core diameters of the atoms constituting the alloys taken from [21], where the weights correspond to the ratios of the respective atoms.

The characteristic range  $1/C$  of the valence-shell overlap repulsion is not known *a priori*. However, its typical values are less sensitive to the atomic composition than the parameters  $\bar{\sigma}$ ,  $A$  and  $B$ . Different atoms have very similar values typically in the range  $C = 1.89 - 4.72 \text{ \AA}^{-1}$  [23].

The latter cannot be easily estimated from first-principles or from literature. Similarly, the prefactor  $B$  of the Born-Mayer term, can be rigorously evaluated only from the exchange integrals of the various overlapping electrons belonging to the valence shells of the two interacting ions. This calculation, even in approximate form, is not feasible except for simple monoatomic crystals. Hence, both  $A$  and  $B$  were taken in our previous analysis as adjustable parameters in the mapping between our schematic logarithmic potential (to be introduced below in Sec.III) and the Ashcroft-Born-Mayer interatomic potential. We shall remark that the Born-Mayer prefactor  $B$  typically has non-trivial large variations from element to element across the periodic table, as shown in many ab initio simulation studies [23, 24]. Consistent with this

known fact, it turns out that  $B$  is the most sensitive parameter in our analysis, in the sense that small variations in  $B$  can lead to large deviations in the fitting of the experimental data. Conversely, the Ashcroft prefactor  $A$  is not a sensitive parameter, and its values are not crucial for the match with experiments.

In Ref. [8], it was found that, in order to fit shear modulus and viscosity data of various alloys, values of the Born-Mayer repulsion strength  $B$  are required which are between two and three orders of magnitude smaller than the Born-Mayer parameters tabulated for pure metals. This important difference has at least two reasons. One reason is that the Born-Mayer formula used for pure substances in the literature is written  $\sim \exp[-Cr]$ , instead of  $\sim \exp[-C(r-\bar{\sigma})]$ , which we use here. Evidently,  $\exp[C\bar{\sigma}] > 1$  partly contributes to explain this discrepancy. However, the fact that  $B$  fitted for multi-component alloys is much smaller than  $B$  found for pure substances is also due to the so-called micro-alloying effect, whereby the addition of even a small amount of different elements with different ionic size and electronic structure induces a strongly nonlinear change in the inter-ionic potential. When there is an atomic size mismatch, this difference intuitively promotes softer repulsion due to the fact that short-ranged packing is more efficient. Of course there could be other important reasons related to the change in electronic structure, e.g. the change in anisotropy of closed electronic shell, which also make the effective short-range repulsion in alloys being effectively milder than in pure metals. Finally, the Born-Mayer parameters in Ref. [25] refer to pairs of atoms, in which the outer electronic structure is clearly much different from metals, where the atoms are significantly ionized.

### III. THE GLOBAL INTERATOMIC REPULSION PARAMETER $\lambda$

In the analysis of Ref. [8], it was found that different disordered alloys can be described by an effective interatomic potential given by Eq.(1) with  $A = 0.3 - 0.5 \text{ eV}$ , and  $B = 5 - 60 \text{ eV}$ . The value of  $\bar{\sigma}$  is uniquely determined by the elemental composition of the alloy, whereas  $q_{\text{TF}} = 1.7 \text{ \AA}^{-1}$  can be kept constant, independent of composition. Furthermore, an even simpler parametrization of the interatomic potential was obtained by mapping Eq.(1) onto a logarithmic expression with a single, global parameter  $\lambda$ , which contains all the information about the steepness (or its inverse, the softness) of the ion-ion repulsion. This simpler expression reads as

$$V(r) = -\lambda \ln(r - 2a_0). \quad (3)$$

The mapping between Eq.(1) and Eq.(3) is shown in Fig.1, for representative parameters of metallic glasses. In all instances examined thus far, Eq.(1) is very accurately represented by Eq.(3).

The main advantage of representing the repulsive part