Atomic volumes of elements: Modern computational methods and experiment

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It is well known that atomic volumes of elements at normal pressure exhibit oscillatory behavior with the rise of atomic number [1, 2]. It was also predicted [2] that the curve of atomic volumes should become monotonic at very high pressures (100 Mbar) due to the disappearance of electron shells. At such pressures semiclassical models are valid; in particular, the Thomas–Fermi model [3] states that all atomic and thermodynamic properties can be described by self-similar relations. It was also shown [4] that molecules are unstable in the Thomas–Fermi approximation so that chemistry is impossible at high enough pressures. In the present work, we apply modern theories to the calculation of atomic volumes at normal and higher pressures. We use pseudopotentials, full-potential density functional theory and average atom models to construct the dependencies of atomic volumes on the atomic number at 1, 10 and 100 Mbar. We compare our calculations with shock-wave experimental data as well as with much more accurate diamond anvil cell measurements. The work is supported by the Russian Science Foundation (grant No. 20-42-04421).

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