Abstract: The boiling point and the elastic modulus are properties which depend on the interaction between the micro-constituents of a substance. We present a possibility to fit a harmonic potential modelling the interaction between molecules of substances whose boiling point is available. The predictive power of a parameter of the potential in the context of microscopic explanation of the elastic modulus is explored statistically for 45 chemical elements. The obtained results can be viewed as a bridge between Fluid and Solid State Theories.

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1. Introduction

It is a challenging task in contemporary Mathematics and Physics to deduce microscopic properties of substances from macroscopic measurements. The success of this kind of deduction depends on whether further macroscopic quantities can be predicted based on the established microscopic model.

In Grycko (2006) a method for fitting the parameters of Lennard-Jones molecular interaction potential is proposed for substances whose boiling point and crystallographic lattice constant are available; therein a possibility of predic-
The notion of Debye temperature from the microscopic model is discussed.

The aim of the present contribution is to demonstrate quantitatively that boiling point and elastic modulus are strongly interrelated through a simple microscopic model of molecular interaction.

The paper is organized as follows. In Section 2 we shortly introduce the notion of elastic modulus; the considerations entail that the elastic modulus depends on the interaction between micro-constituents of a substance. In Section 3 we propose a method for fitting a parameter $D$ of harmonic interaction potential $\Psi$ to the boiling point. Parameter $D$ serves in Section 4 as a physically interpretable regressor for the explanation of the values of the elastic modulus $E$ for 45 chemical elements. The considerations reveal a strong correlation between $D$ and $E$ which motivates the introduction of two universal physical constants enabling us to interrelate quantitatively the boiling point with the elastic modulus.

2. The Notion of Elastic Modulus

If two opposite forces of strength $F$ act on the ends of a rod of initial length $L_0$, then the length $L$ of the rod increases according to

$$F = c \cdot (L - L_0)$$

(2.1)

where constant $c$ depends on the material and on the geometry of the rod. (2.1) is called Hooke’s law.

Let $A$ denote the cross area of the rod. Hooke’s law implies the relation

$$\frac{F}{A} = E(X) \cdot \frac{L - L_0}{L_0}$$

(2.2)

where constant $E(X)$ is specific for substance $X$ constituting the rod. $E(X)$ is called elastic modulus of $X$; in the present contribution we neglect the dependence of $E(X)$ on temperature.
2. Fitting Harmonic Potential to the Boiling Point

Let \( T_c(X) \) and \( \varrho_c(X) \) denote the critical temperature and the critical density of substance \( X \), respectively. Motivated by the fact that critical data are sometimes not available, the approximation

\[
T_c(X) = \alpha \cdot T_B(X)
\]

is proposed in Grycko (2006); \( T_B(X) \) denotes the standard boiling point of substance \( X \) and \( \alpha = 1.7759 \) is an universal constant.

In Grycko (2005) the general formula

\[
\frac{1}{5^{1/2}} \cdot \left( \frac{3}{4\pi \varrho_c(X)} \right)^{1/3} \cdot \left( \frac{k_B T_c(X)}{m_r(X) N_A} \right)^{1/2} = \frac{\hbar}{2}
\]

is motivated and statistically confirmed where \( k_B = 1.38 \cdot 10^{-23} \text{J/K} \) and \( \hbar = 1.05 \cdot 10^{-34} \text{Js} \) denote the Boltzmann and Planck constant, respectively, \( N_A = 6.02 \cdot 10^{26} \text{kg}^{-1} \) is the modified Avogadro number and \( m_r(X) \) denotes the relative molecular mass of substance \( X \). Equation (3.2) interrelates critical temperature with critical density.

Combining (3.1) and (3.2) yields an approximation of critical data \( T_c(X) \) and \( \varrho_c(X) \) for every substance \( X \) whose boiling point \( T_B(X) \) and relative molecular mass \( m_r(X) \) are available.

The interaction between atoms of the noble gas Ar is modelled by the Lennard-Jones interaction potential \( \Phi_{Ar} \) (cf. Bergmann, Schaefer (1992))

\[
\Phi_{Ar}(r) = 4U_{Ar} \cdot \left( \left( \frac{r_{Ar}}{r} \right)^{12} - \left( \frac{r_{Ar}}{r} \right)^6 \right)
\]

with parameter values

\[
U_{Ar} = 120.0 \text{K} \cdot k_B \quad \text{and} \quad r_{Ar} = 3.4 \cdot 10^{-10} \text{m}.
\]

According to the principle of corresponding states the quantities

\[
\lambda_U := \frac{U_X}{k_B T_c(X)} \quad \text{and} \quad \lambda_\varrho := r_X \cdot \varrho_c(X)^{1/3}
\]
are universal where $U_X$ and $r_X$ denote the parameters of Lennard-Jones potential

\begin{equation}
\Phi_X(r) = 4U_X \cdot \left( \left( \frac{r_X}{r} \right)^{12} - \left( \frac{r_X}{r} \right)^6 \right)
\end{equation}

describing the interaction between molecules of substance $X$. From the critical data for Ar and from (3.4) we obtain

\begin{equation}
\lambda_U = 0.7740 \quad \text{and} \quad \lambda_\varrho = 0.9459.
\end{equation}

Therefore we are able to fit parameters $U_X$ and $r_X$ of Lennard-Jones potential $\Phi_X$ for every substance $X$ whose boiling point $T_B(X)$ and relative molecular mass $m_r(X)$ are known.

In order to approximate $\Phi_X$ by the harmonic potential

\begin{equation}
\Psi_X(r) = \frac{1}{2} \cdot D_X(r - r_m(X))^2
\end{equation}

we put

\begin{equation}
D_X := \Phi_X''(r_m(X))
\end{equation}

where $r_m(X) = 2^{1/6} \cdot r_X$ denotes the distance between two molecules at which $\Phi_X$ is minimal. (3.9) entails the equality of the first and second derivatives of $\Phi_X$ and $\Psi_X$ at $r_m(X)$.

If boiling point $T_B(X)$ and relative molecular mass $m_r(X)$ are known for a substance $X$, then we can approximate the interaction between molecules of $X$ by harmonic potential $\Psi_X$ where constant $D_X$ is given according to (3.9).

4. The Statistical Evaluation

Based on the data $T_B(X)$ and $m_r(X)$ for 45 chemical elements $X$ whose elastic moduli are available, the values of parameter $D_X$ of the harmonic potential $\Psi_X$ can be computed according to Section 3. $D_X$ is the strength of interaction between adjacent molecules of substance $X$. 

4
In the present section we explore statistically the predictive power of $D_X$ w.r.t. elastic modulus $E(X)$. In Figure 1 the horizontal axis corresponds to the values of parameter $D_X$ of molecular interaction and the vertical axis to the values of $\ln(E(X))$ for 45 chemical elements $X$. The visual impression suggests a linear dependence between $D_X$ and $E(X)$. After removal of the outliers Be, Ir, Li and Ru the empirical correlation coefficient attains the value 0.8512 which confirms the fact that $D_X$ carries valuable statistical information about the interaction between molecules of substance $X$; parameter $D_X$ can serve as a physically plausible and microscopically interpretable regressor. This motivates the ansatz

(4.1) \[ E(X) = \gamma_0 + \gamma_1 \cdot D_X \]

for microscopic explanation of elastic modulus $E(X)$. Solving (4.1) by the least-squares method yields the estimates

(4.2) \[ \hat{\gamma}_0 = 3.9592 \cdot 10^{10} \text{N/m}^2 \quad \hat{\gamma}_1 = 1.3416 \cdot 10^8 \text{m}^{-1}. \]

Parameters $\gamma_0$ and $\gamma_1$ are universal physical constants. On the occasion of the 70th birthday of Professor Otto Moeschlin from Hagen we call the constant

\[ \lambda_M := \gamma_1^{-1} \]
Moeschlin universal length. A statistical approximation of $\lambda_M$ based on (4.2) is given by

$$\hat{\lambda}_M = 7.4539 \cdot 10^{-9} \text{m}.$$  

The statistical considerations of the present section suggest that there is a quantitative interrelation between boiling point and elasticity modulus which can be viewed as a bridge between Fluid and Solid State Theories. We believe that the prediction of the elastic modulus can be improved if more sophisticated microscopic models are applied; this would, however, require the implementation and carrying out of long term computer experiments.

References

