

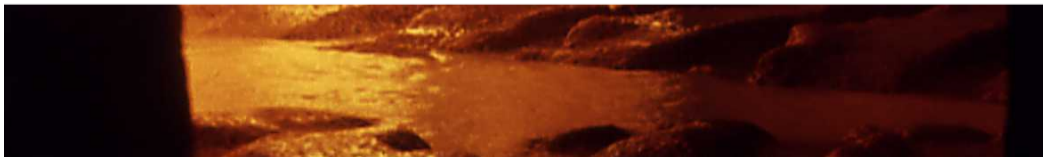


Physical-informed machine learning prediction of properties of oxide glasses

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1. Industrial context



L'ORÉAL
GROUPE

1
THE WORLD
LEADER
IN BEAUTY

ULTRA LIGHT GLASS BOTTLE

Resistant

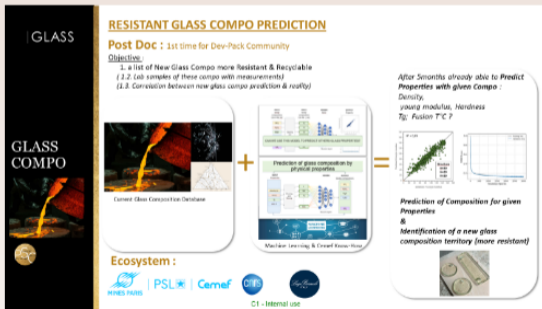
**Recyclable
Eco-Desirable**

**L'Oréal R&D Project
with CEMEF**



Resistant & Recyclable Glass Composition
Glass Scientist, Machine Learning, Genetic AI

Cemef : F. Pigeonneau, Elie Hachem



1. Industrial context

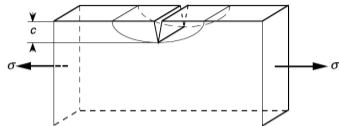


Figure 1: Tensile experiment on a sample with a size flaw c .

$$\sigma_c = \frac{\sqrt{2E\gamma}}{\sqrt{\pi c}}. \quad (1)$$

The fracture toughness is defined¹:

$$K_{Ic} = \sqrt{2E\gamma}, \text{ in plane-stress,} \quad (2)$$

$$K_{Ic} = \sqrt{\frac{2E\gamma}{1-\nu^2}}, \text{ in plane-strain.} \quad (3)$$

¹A. A. Griffith: The Phenomena of Rupture and Flow in Solids, in: *Philos. Trans. R. Soc. Lond. Ser. A* 1921.

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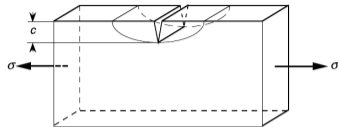


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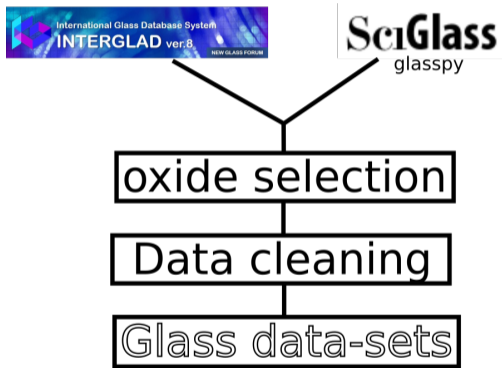
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Mechanical properties vs glass composition

¹Griffith: The Phenomena of Rupture and Flow in Solids (see n. 1).

1. Industrial context
2. Deep learning method
3. Density & molar volume
4. Young's modulus & packing factor
5. Poisson coefficient
6. Synthesis & perspectives

2. Deep learning method



- i) **network formers:** SiO_2 , B_2O_3 , P_2O_5 , V_2O_5 and GeO_2 ;
 - ii) **network modifiers:** Na_2O , K_2O , Li_2O , CaO , MgO , SrO , BaO , Fe_2O_3 , Y_2O_3 , La_2O_3 ;
 - iii) **network intermediates:** Al_2O_3 , TiO_2 , ZrO_2 , ZnO and PbO .
- ▶ keras of Python ➔ Artificial Neural Networks (ANN) with 2 or 3 hidden layers with 20 neurons.
 - ▶ The Gaussian error linear units “gelu” activation function (hidden layers) and linear function for output layer.
 - ▶ Adam solver used for the optimization.
 - ▶ Variable to fit is normalized.
 - ▶ Spitting of training, validation and test sub-sets is [0.6; 0.2, 0.2].

3. Density & molar volume

- ▶ According to Huggins² and Huggins and Sun³ for a glass of N oxides $M_{n_i}O_{m_i}$:

$$\frac{1}{\rho} = \sum_{i=1}^N [(k + b_{\text{SiO}_2}) n_i + m_i c_i] \frac{y_i}{\mathcal{M}_i}, \quad (4)$$

- ▶ After changing y_i in x_i :

$$\mathcal{V}_{\mathcal{M}} = \sum_{i=1}^N [(k + b_{\text{SiO}_2}) n_i + m_i c_i] x_i. \quad (5)$$

²M. L. Huggins: The Density of Silicate Glasses as a Function of Composition, in: *J. Opt. Soc. Am.* 30.9 (1940), pp. 420–430.

³M. L. Huggins/K.-H. Sun: Calculation of density and optical constants of a glass from its composition in weight percentage, in: *J. Am. Ceram. Soc.* 26.1 (1943), pp. 4–11.

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ANN model on \mathcal{V}_M

²Huggins: The Density of Silicate Glasses as a Function of Composition (see n. 2).

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3. Density & molar volume

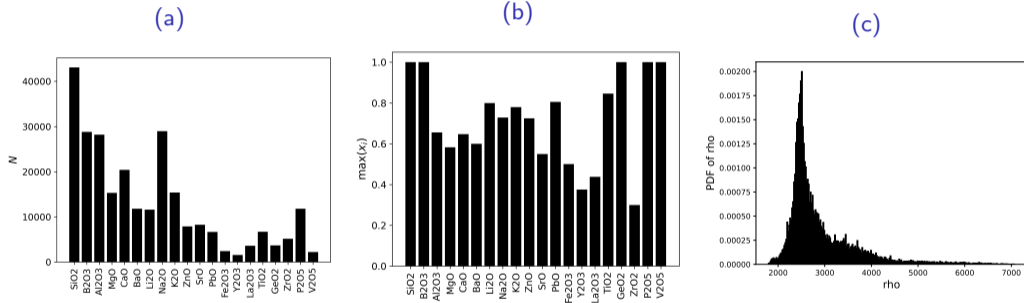


Figure 2: Histograms of (a) glasses and (b) $\max(x_i)$ in the ρ data-set of 64 420 glasses, (c) pdf of ρ in kg/m³.

3. Density & molar volume

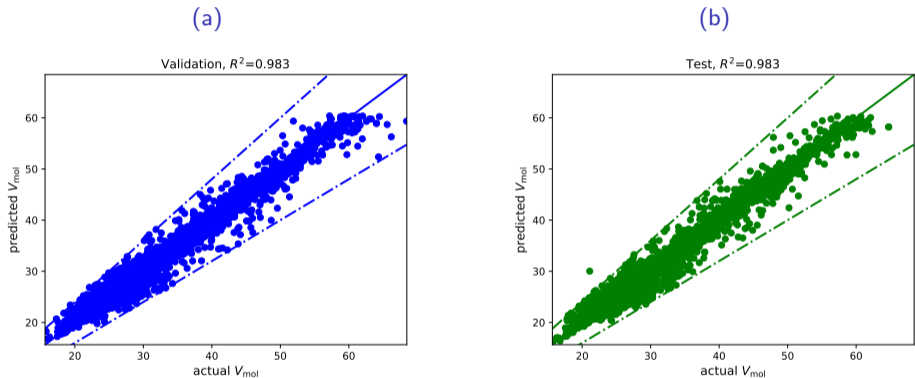


Figure 3: Predicted \mathcal{V}_M in (cm^3/mol) as a function of data-set values for (a) the validation sub-set and (b) the test sub-set.

3. Density & molar volume

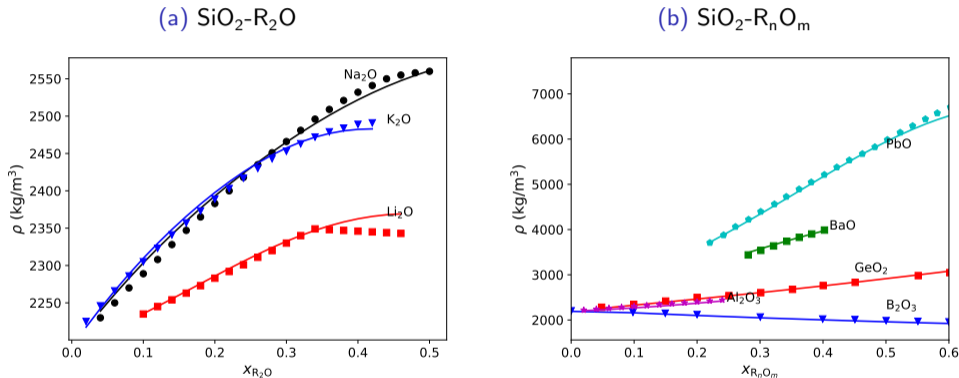


Figure 4: ρ (kg/m³) of (a) alkaline glasses and (b) $\text{SiO}_2\text{-R}_n\text{O}_m$ glasses. Symbols are experimental data according to Bansal and Doremus⁴.

⁴N. P. Bansal/R. H. Doremus: Handbook of Glass Properties, 1986.

4. Young's modulus & packing factor

- ▶ According to Makishima & Mackenzie⁵, E is given by

$$E = 2V_t\mathcal{G}, \quad (6)$$

$$V_t = \frac{\sum_{i=1}^N V_i x_i}{\mathcal{V}_{\mathcal{M}}}, \quad (7)$$

$$\mathcal{G} = \sum_{i=1}^N G_i x_i. \quad (8)$$

- ▶ G_i taken from data of Inaba et al.⁶.

⁵A. Makishima/J. D. Mackenzie: Direct calculation of Young's modulus of glass, in: *J. Non-Cryst. Solids* 12.1 (1973), pp. 35–45.

⁶S. Inaba/S. Fujino/K. Morinaga: Young's Modulus and Compositional Parameters of Oxide Glasses, in: *J. Am. Ceram. Soc.* 82.12 (1999), pp. 3501–3507.

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V_t determined from a deep learning method on E data-set

⁵Makishima/Mackenzie: Direct calculation of Young's modulus of glass (see n. 5).

⁶Inaba/Fujino/Morinaga: Young's Modulus and Compositional Parameters of Oxide Glasses (see n. 6).

4. Young's modulus & packing factor

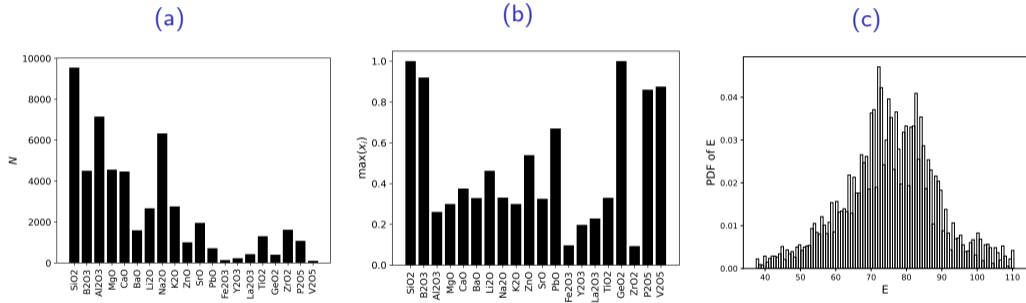


Figure 5: (a) number of glasses and (b) $\max(x_i)$ in the data-set of E of 10 846 glasses, (c) pdf of E in GPa.

4. Young's modulus & packing factor

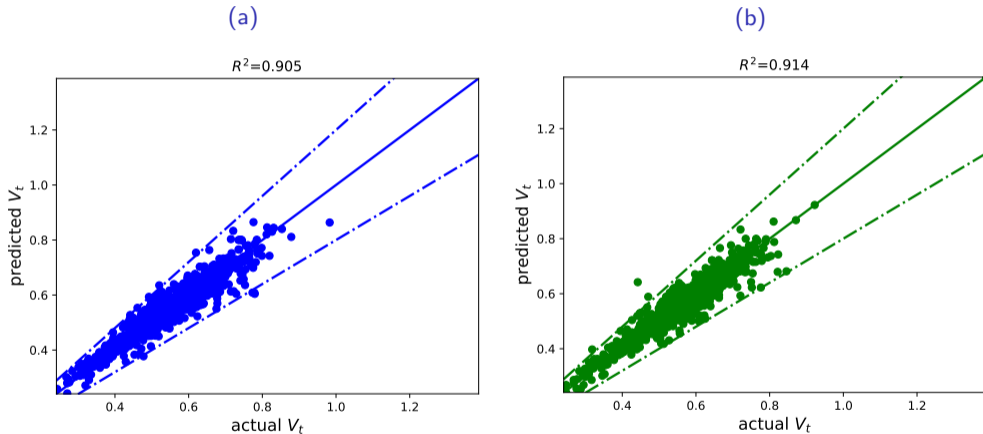


Figure 6: Predicted \mathcal{V}_t as a function of data-set values for the (a) validation sub-set and (b) test sub-set.

4. Young's modulus & packing factor

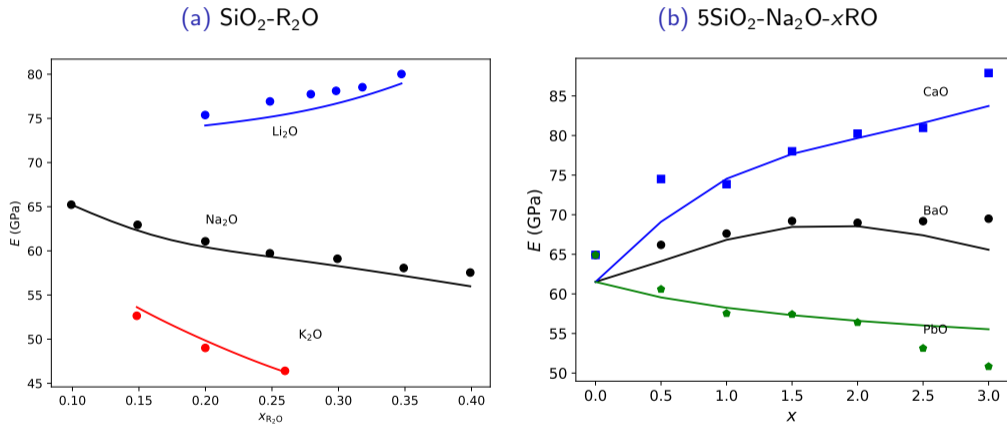


Figure 7: E in (a) $\text{SiO}_2\text{-R}_2\text{O}$ and (b) $5\text{SiO}_2\text{-Na}_2\text{O-xRO}$. Data taken in⁷.

⁷A. K. Varshneya/J. C. Mauro: Fundamentals of Inorganic Glasses, Third, 2019.

5. Poisson coefficient

- ▶ According to Makishima & Mackenzie⁸, ν is given by

$$\nu = \frac{1}{2} - \frac{1}{6\alpha V_t}, \quad (9)$$

- ▶ $\alpha=1.2$ in Makishima & Mackenzie (1975).
- ▶ Rocherulle et al.⁹ proposed $\alpha=1.08$

⁸A. Makishima/J. D. Mackenzie: Calculation of bulk modulus, shear modulus and Poisson's ratio of glass, in: J. Non-Cryst. Solids 17 (2 1975), pp. 147–157.

⁹J. Rocherulle et al.: Elastic moduli of oxynitride glasses: Extension of Makishima and Mackenzie's theory, in: J. Non-Cryst. Solids 108.2 (1989), pp. 187–193.

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ANN model on α

⁸Makishima/Mackenzie: Calculation of bulk modulus, shear modulus and Poisson's ratio of glass (see n. 8).

⁹Rocherulle et al.: Elastic moduli of oxynitride glasses: Extension of Makishima and Mackenzie's theory (see n. 9).

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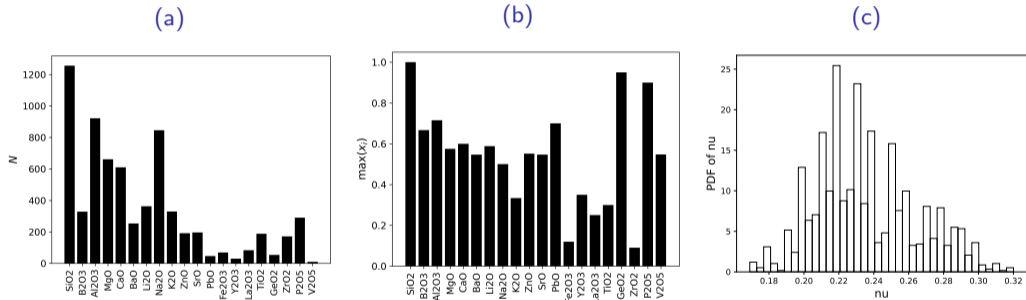


Figure 8: (a) number of glasses and (b) $\max(x_i)$ in the data-set of ν of 1464 glasses, (c) pdf of ν .

5. Poisson coefficient

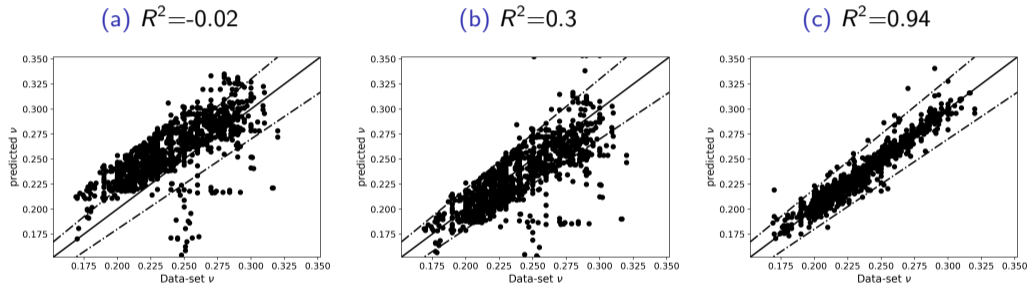


Figure 9: Comparison of the computation of ν with the data-set for (a) $\alpha=1.2$, (b) $\alpha=1.08$ (c) α from ANN model.

5. Poisson coefficient

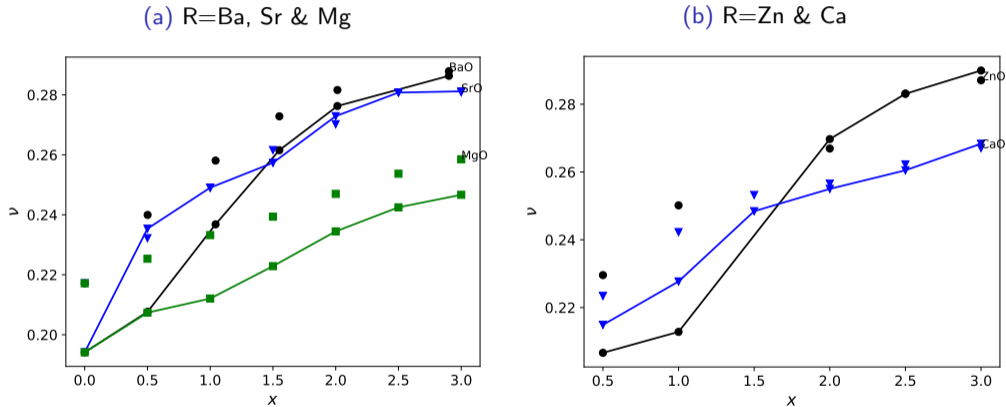


Figure 10: ν in $5\text{SiO}_2\text{-Na}_2\text{O-xRO}$. Data taken in¹⁰.

¹⁰Varshneya/Mauro: Fundamentals of Inorganic Glasses (see n. 7).

6. Synthesis & perspectives

Synthesis

- ▶ Creation of data-sets with a large amount of glasses (two databases have been used);
- ▶ Deep learning method applied to determine mechanical properties;
- ▶ Coupling with theoretical models enhances the accuracy of the prediction;
- ▶ Developments of model for T_m ($\log(\eta)=1$), T_s ($\log(\eta)=6.65$), and T_g ($\log(\eta)=12$) (η in Pa · s).

6. Synthesis & perspectives

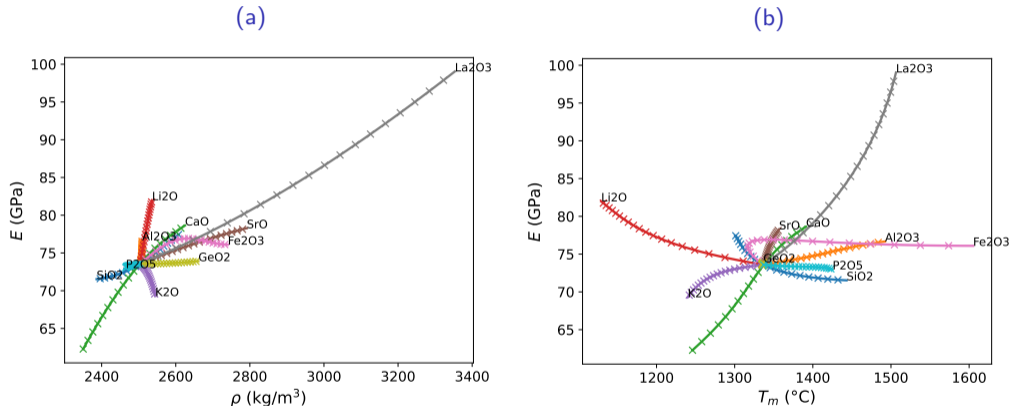


Figure 11: Spider-graph with a based composition ($0.74\text{SiO}_2-0.13\text{Na}_2\text{O}-0.13\text{CaO}$): (a) E vs. ρ and (b) E vs. T_m .

6. Synthesis & perspectives

Perspectives

- ▶ Extend the work to K_{Ic} and γ the fracture surface energy;
- ▶ Determination of glass compositions based on genetic algorithm;
- ▶ Introduce probability aspect to determine prediction uncertainties.

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Thank you for your attention!