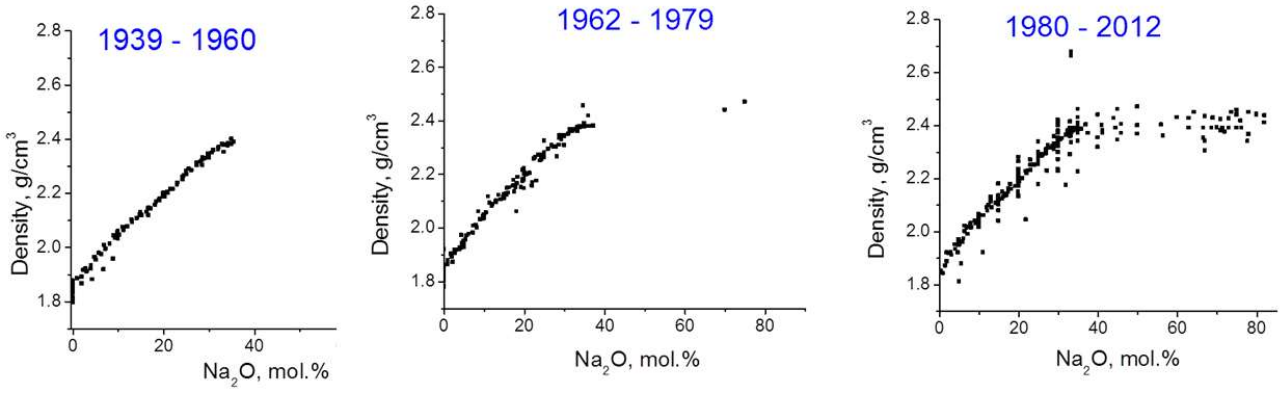
# Evaluation of Quality of Measured Property Data by Using the Qualimetric Approach

## Contents

## Challenges

1. During last decades, the quality of published glass property data reduced and the number of erroneous data greatly increased. Here you see only one example requiring no comments. How to fight?




*Density data for glasses in the system $Na_2O$-$B_2O_3$ published in different time periods*

2. New experimental investigations require much time and cost. There are many calculation methods allowing prediction of multiple glass properties from chemical compositions in rather wide areas. However, the accuracy of such calculations considerably depends on composition areas, and it is not an easy task to evaluate the errors of calculation for a particular composition.

How to evaluate the errors of calculations? What to do if several methods give contradictory results?

Only one example: Young's modulus of an aluminoborosilicate glass. What to trust?

| Component | Mol.% |
|---|---|
| Na2O | 5 |
| CaO | 5 |
| $Al_2O_3$ | 10 |
| $B_2O_3$ | 10 |
| $SiO_2$ | 70 |

| Author(s) of method | Calculated E (GPa) |
|---|---|
| Appen | 63.5 |
| Demkina | 75.6 |
| Gan Fuxi | 66.2 |
| Kozlovskaya | 79.4 |
| Priven (2000) | 74.0 |
| Priven (1998) | 72.9 |
| Winkelmann and Schott | 81.3 |

## Approach

Experimental and calculated values of a property for glasses of similar compositions should "cross-validate" each other:

- *Available experimental data determine quality of calculation methods;*
- *Best calculation methods determine quality of new experimental data.*

Similar approach is used in qualimetry – a scientific discipline that determines numerical measure for quality by statistical treatment of independent evaluations of multiple objects. That is why our method is named "qualimetric".

## How it works?

The procedure in general is as follows:

1. Select experimental property data for glasses of similar compositions
    - From 15 to 50 data points are selected
    - Minimum 2 data sources
    - Not more than 70% of data from single source
2. Rank the calculation methods by accuracy
    - Criterion: standard deviations of calculation results from selected experimental data $S_i$ ($i$ is the index of method)
    - Weight factors of methods: $W_i = \frac{1/{S_i}^2}{\sum_k 1/{S_k}^2}$
3. Calculate the most probable property value and its confidence limit for a given glass
    - Most probable property value: $P_{calc} = \sum_i (P_i W_i)$
    - Confidence interval ($p$=0.95): 2σ where $\sigma = \frac{1}{\sqrt{\sum_i 1/{S_i}^2}}$

## Example

Consider the same example: Young's modulus of an aluminoborosilicate glass (composition is specified above). The results of calculation are as follows:

| Method | Result | Standard deviation |
|---|---|---|
| Appen | 63.54 | 8.7 |
| Clarke et al. | - | - |
| Demkina-76 | 75.63 | 11 |
| Gan Fuxi-74 | 66.17 | 4.3 |
| Kozlovskaya | 79.39 | 11 |
| Makishima and Mackenzie | - | - |
| Priven-2000 | 73.99 | 11 |
| Priven-98 | 72.90 | 11 |
| Winkelmann and Schott | 81.63 | 9.6 |

***Most probable value and its confidence interval: 70.15±8.6 GPa***

## What are the benefits?

1. For a particular composition, we have:
    a. the most probable value, more accurate than each particular prediction (if two or more methods are available);
    b. the confidence limit that evaluates the quality of calculation.
2. We can evaluate the quality of published data.
    In particular, we can find the suspicious data points that greatly deviate from independently measured data and results of calculations.

## Suggested service

We suggest a new service: **evaluation of most probable values and their confidence limits for glass properties.**

### What you specify:

- Chemical composition of glass
- One or more properties to evaluate
- Temperature or temperature range for each property

### What you get:

1. Most probable value(s) of selected property (-ies)
2. Confidence limit(s)
3. In the case if calculation is impossible or confidence limit is outside the average level (see the values in the Appendix below), suggestion of glass of closest composition for which the most

probable value is determined with acceptable accuracy. You could synthesize this glass, measure its property and make you sure that your experiment in general is accurate enough.

## Price

- 20 US dollars for an order, plus 10 US dollars for each data point.

Note: A "data point" means one property at one temperature for one glass composition. Prices are valid until September 30, 2013.

## Procedure

A customer specifies chemical composition(s) and property (-ies) to evaluate by email to sciglass@itcwin.com. SciGlass team calculates the price according to the above-described rule, analyzing the possibility of calculations for your particular case and sends a quote. After payment, the results are to be sent to the Customer.

## Limitations

In some specific composition areas where no experimental data are available and no calculation methods exist for a given property, the qualimetric method cannot be applied. In particular, there are no calculation methods for oxy-halide and oxy-chalcogenide glasses. For such cases, we only can suggest a glass of simpler (but closest) composition to evaluate the quality of your experiments.

## Appendix

### List of calculated properties (can be extended)

- Density at room temperature
- Thermal properties:
  - Thermal expansion coefficient below $T_g$
  - Heat capacity (20…1400$^{o}$C)
  - Thermal conductivity (*silicate systems only)*
- Optical properties:
  - Refractive index $n_d$
  - Mean dispersion
  - Abbe's number
- Mechanical properties:
  - Young's modulus
  - Shear modulus
- Surface tension above $T_g$
- Viscosity
- Glass transition temperature $T_g$ (*for standard thermal schedule: heating with the rate 3…20 K/min after cooling with similar rate*)

### Average values of accuracy for different properties

| Property | Unit | Accuracy |
|---|---|---|
| **Density @ 20oC** | $g/cm^3$ | 0.05 |
| **Thermal expansion coefficient** | $K^{-1}$ | 5E-7 |
| **Heat capacity @ 20oC** | J/kg*K | 45 |
| **Refractive index nd** | | 0.01 |
| **Mean dispersion** | | 7E-4 |
| **Young's modulus** | GPa | 5 |
| **Shear modulus** | GPa | 2 |
| **Tg** | $^oC$ | 37 |
| **Littleton point** | $^oC$ | 30 |
| **T13** | $^oC$ | 20 |
| **T3** | $^oC$ | 35 |
| **TK-100** | $^oC$ | 37 |
| **logEta at 1200oC** | log(P) | 0.23 |
| **Surface tension at T>Tg** | $mJ/m^2$ | 20 |

## Links for more details

### *Reports in the XXI International Congress on Glass (Prague, 2013)*

O. Mazurin and A. Priven. On the Ways Reliable Values of Glass Properties Should Be Prepared for Publishing

A. Priven and O. Mazurin. Qualimetric Approach to Evaluation of the Accuracy of Glass Property Measurements

### *Examples*

Examples of erroneous data found in the literature

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