

Supporting Information

Network Former Mixing (NFM) Effects in Alkali Germanotellurite Glasses.

Henrik Bradtmüller¹, Ana Candida Martins Rodrigues², Hellmut Eckert^{1,3,a,b}

¹Institut für Physikalische Chemie, Westfälische Wilhelms-Universität, Corrensstr. 30, D-48149, Münster, Germany

²Universidade Federal de São Carlos, Departamento de Engenharia de Materiais, CP 676, 13565-905, São Carlos, SP, Brasil

³Instituto de Física de São Carlos, Universidade de São Paulo, Av. Trabalhador São-carlense 400 São Carlos, S.P., 13566-590, Brasil

* Corresponding author:

Email ^a: eckert@ifsc.usp.br; Ph: +55-16-3373-8775

Email ^b: eckerth@uni-muenster.de

Table S1 – Nominal chemical compositions (nom.) of the $(\text{A}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ (A = Li, Na) glass samples and those measured by ICP-OES, XRF and EDS. TeO_2 and GeO_2 contents determined by XRF and EDS for the A = Li glasses were normalized assuming the respective Li_2O contents from ICP-OES or the nominal ones when the latter method was not applied. All the values are given in mass percent (m%). The errors are 0.5, 1 and 2 m% for ICP-OES, XRF and EDS respectively.

Composition		m%(A_2O)				m%(TeO_2)			m%(GeO_2)		
		nom.	XRF	EDS	ICP-OES	nom.	XRF	EDS	Nom.	XRF	EDS
A = Li	$x = 0.0$	10.9	-	-	11.1	0.0	0.0	0.0	89.1	90.0	90.0
	$x = 0.2$	10.0	-	-	n.A.	24.9	23.4	25.1	65.2	67.6	65.8
	$x = 0.4$	9.2	-	-	9.7	45.8	44.4	46.7	45.0	46.8	44.4
	$x = 0.5$	8.8	-	-	n.A.	55.1	54.4	57.1	36.1	37.5	34.8
	$x = 0.6$	8.5	-	-	7.9	63.7	63.8	65.1	27.8	28.8	27.5
	$x = 0.8$	7.9	-	-	n.A.	79.1	78.9	79.5	13.0	13.7	13.1
	$x = 1.0$	7.4	-	-	7.1	92.6	93.3	93.3	0.0	0.0	0.0
A = Na	$x = 0.0$	20.2	n.A.	14.6	-	0.0	n.A.	0.0	79.8	n.A.	85.4
	$x = 0.2$	18.7	13.4	15.3	-	22.4	22.0	22.7	58.9	64.6	62.1
	$x = 0.4$	17.3	14.1	14.2	-	41.7	43.9	42.4	41.0	42.0	43.4
	$x = 0.5$	16.7	15.1	n.A.	-	50.3	46.7	n.A.	33.0	38.2	n.A.
	$x = 0.6$	16.2	13.5	12.2	-	58.3	61.0	62.2	25.5	25.5	25.7
	$x = 0.8$	15.2	11.6	16.2	-	72.9	78.6	74.2	11.9	9.8	9.6
	$x = 1.0$	14.3	12.3	12.4	-	85.7	87.7	87.5	0.0	0.0	0.0

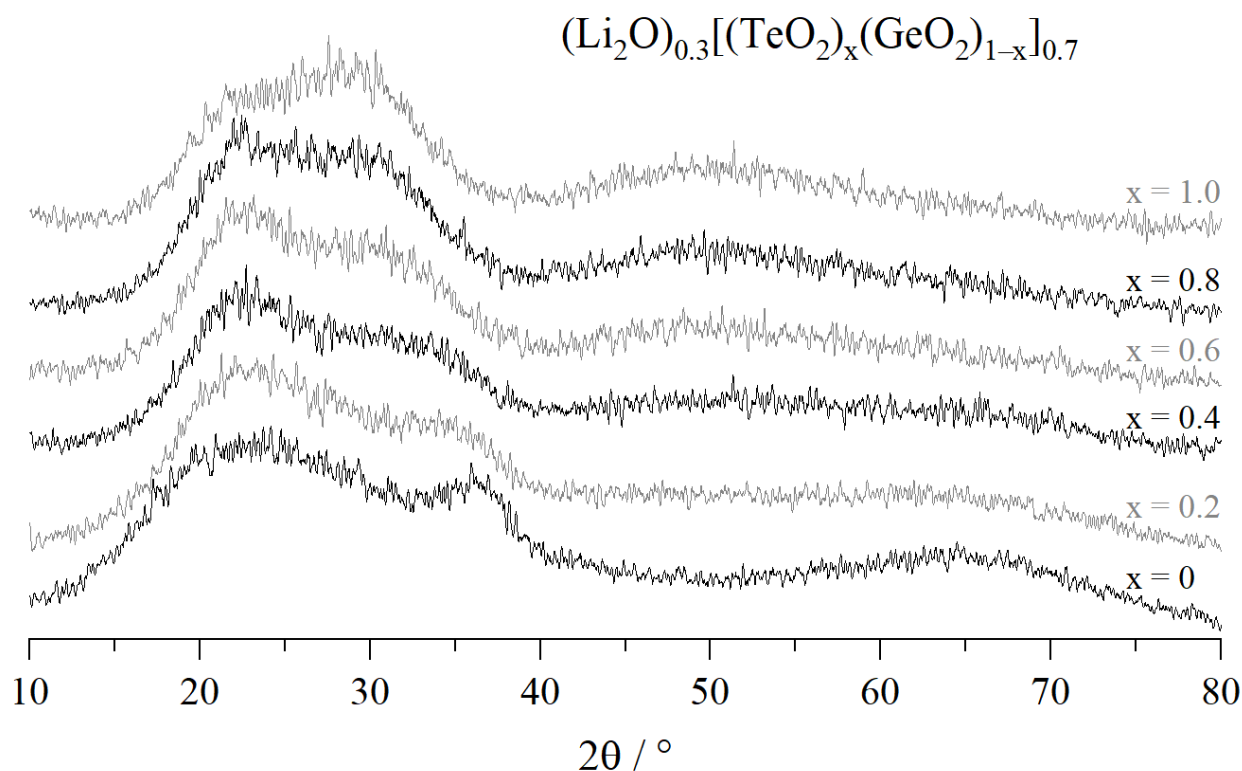


Figure S1: Powder X-ray diffractograms of $(\text{Li}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ glasses.

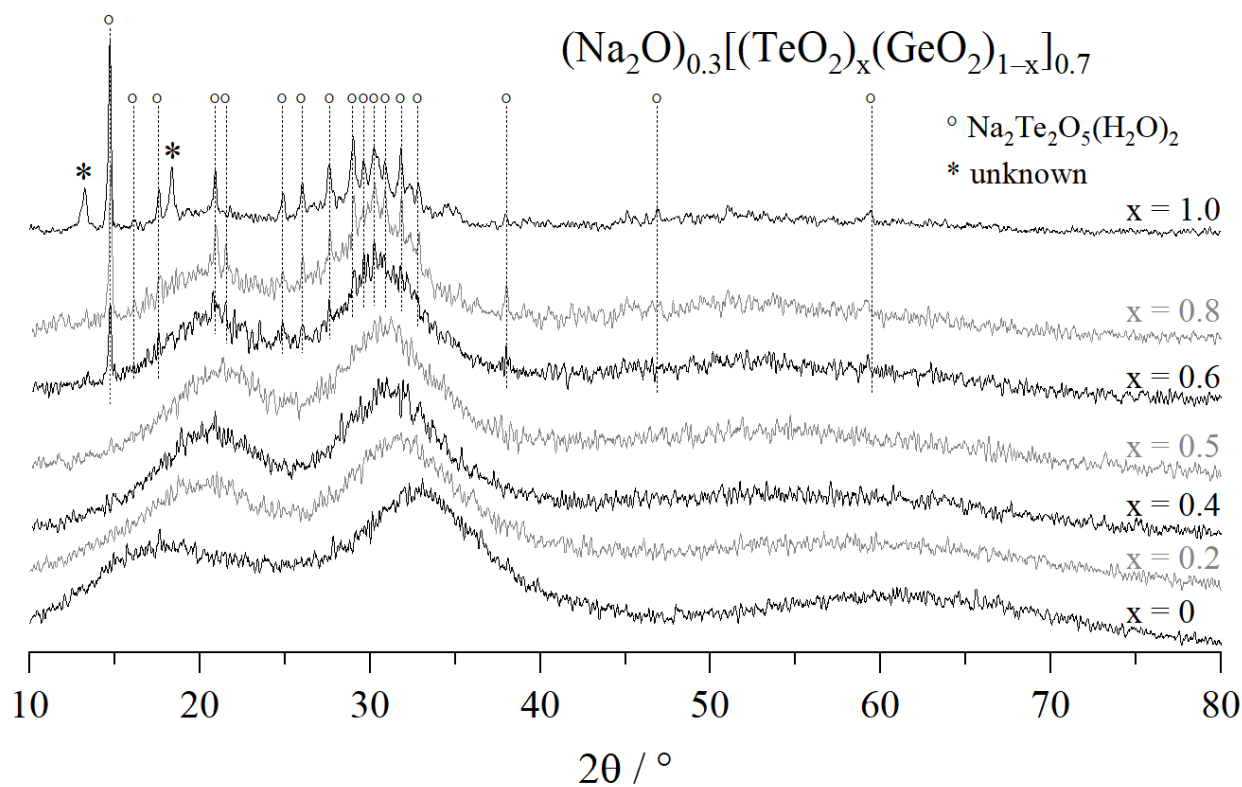


Figure S2: Powder X-ray diffractograms of $(\text{Na}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ glasses. Asterisks, circles, and dashed vertical lines indicate diffraction bands attributable to crystalline phases found with help of the Qualx2 software[1] using the crystallography open database (COD).[2]

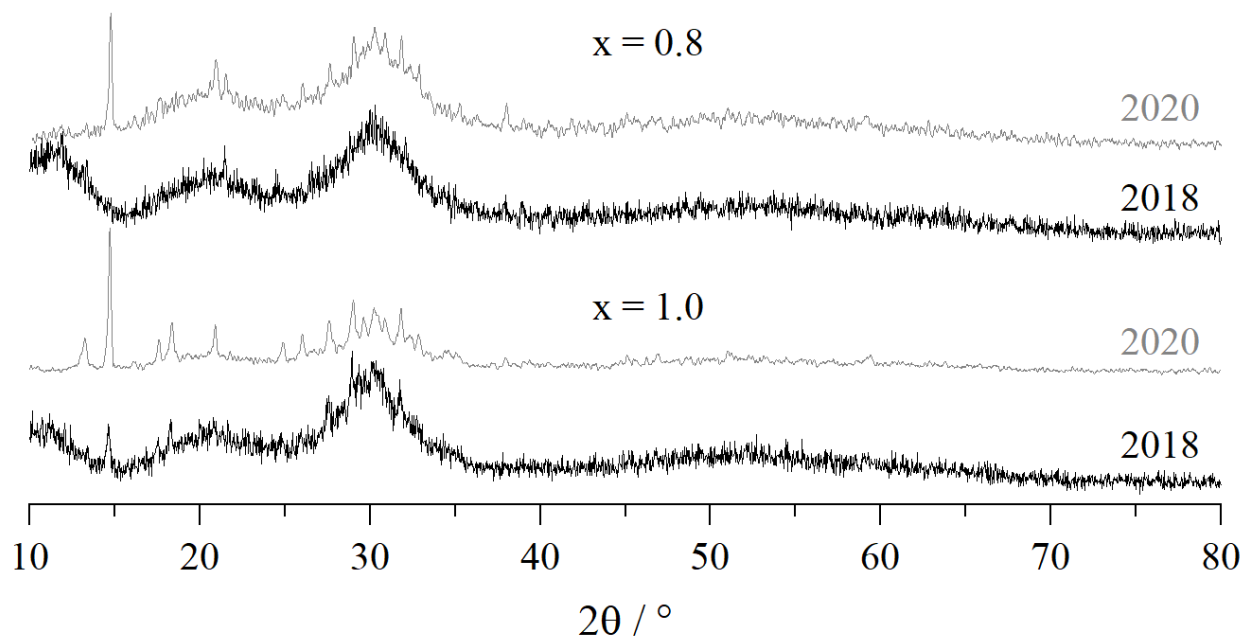


Figure S3: Comparison of powder X-ray diffractograms of $(\text{Na}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ glasses with $x = \{0.8; 1.0\}$, recorded shortly after preparation (2018) and two years later (2020). Visible diffraction bands are attributable to $\text{Na}_2\text{Te}_2\text{O}_5(\text{H}_2\text{O})_2$ (see also Figure S2).

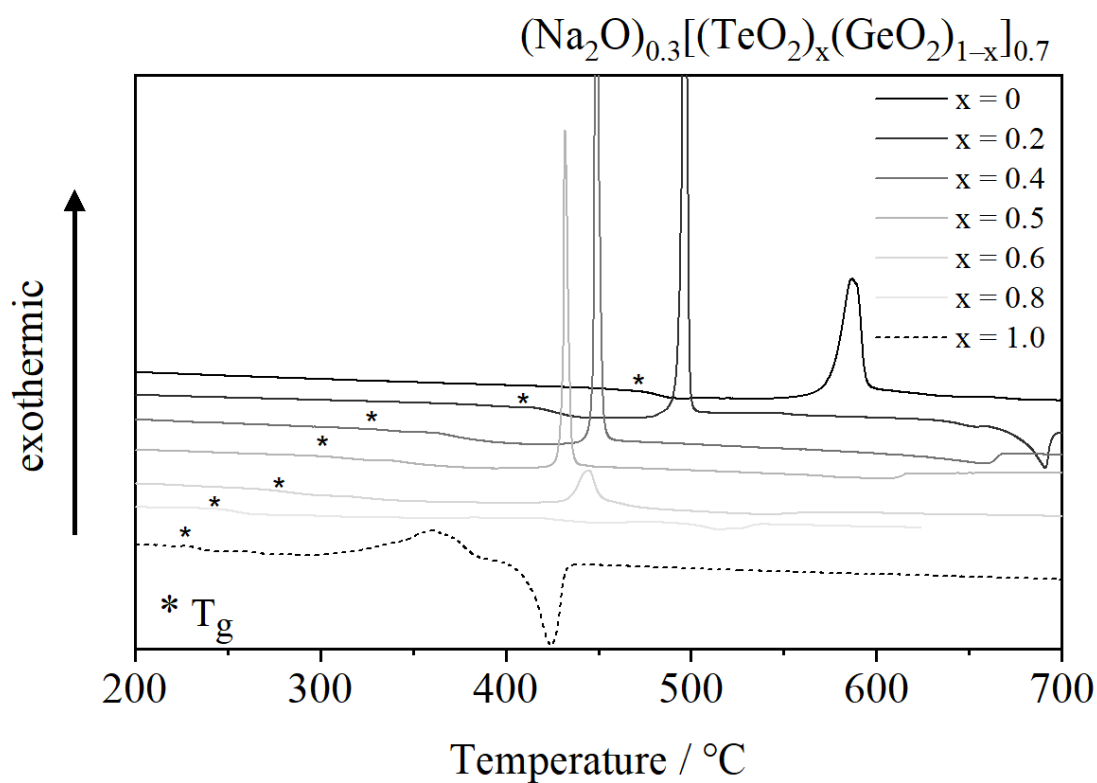
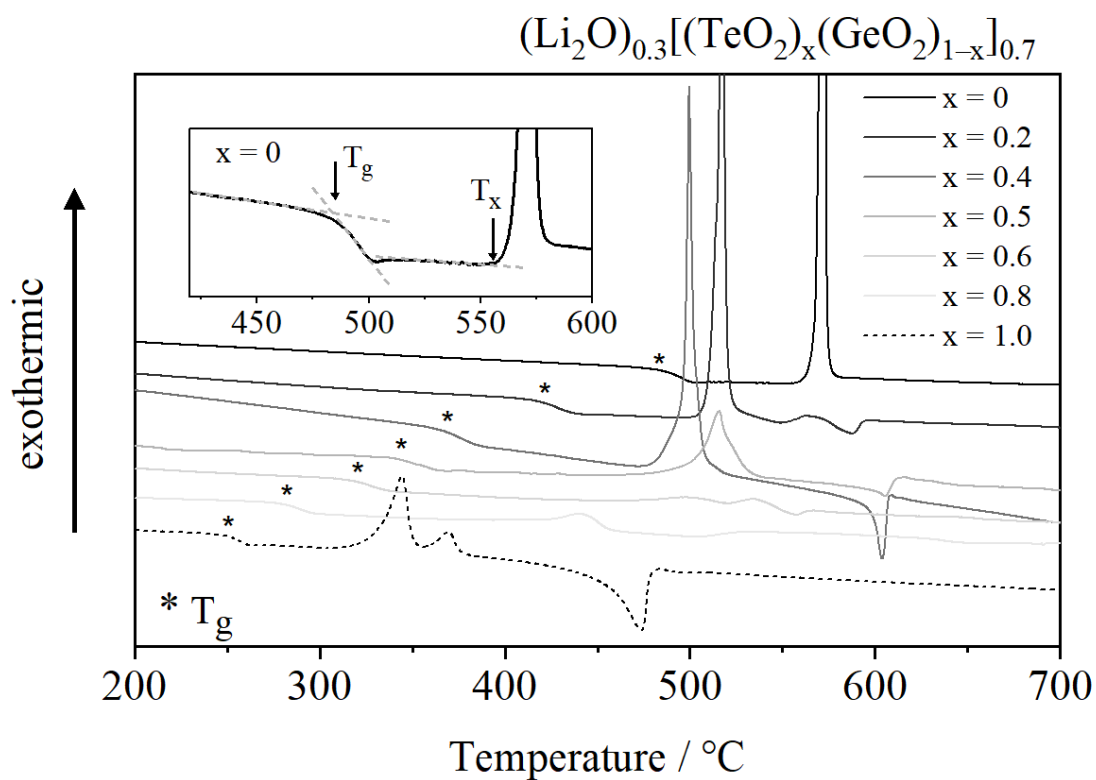


Figure S4: DSC curves of $(\text{A}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ ($\text{A} = \text{Li}, \text{Na}$) glasses. The inset (top) shows exemplarily the extraction of characteristic temperatures T_x and T_g (indicated by asterisks).

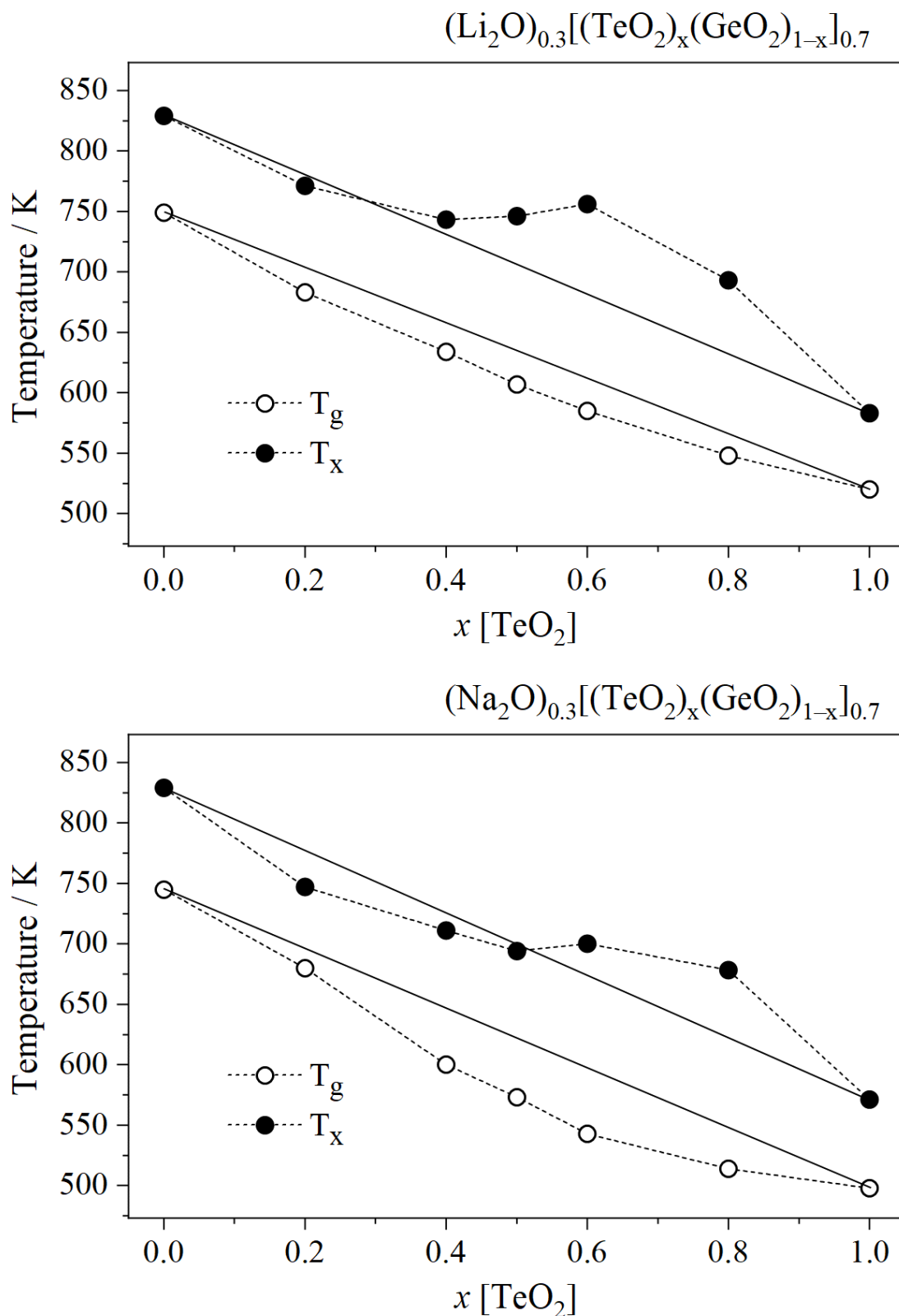


Figure S5: Characteristic temperatures T_x and T_g of $(\text{A}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ ($\text{A} = \text{Li}, \text{Na}$) glasses against glass composition x . Solid lines serve as guide to the eye and connect the values of endmember compositions $x = 0$ ($(\text{A}_2\text{O})_{0.3}(\text{GeO}_2)_{0.7}$) and $x = 1$ ($(\text{A}_2\text{O})_{0.3}(\text{TeO}_2)_{0.7}$).

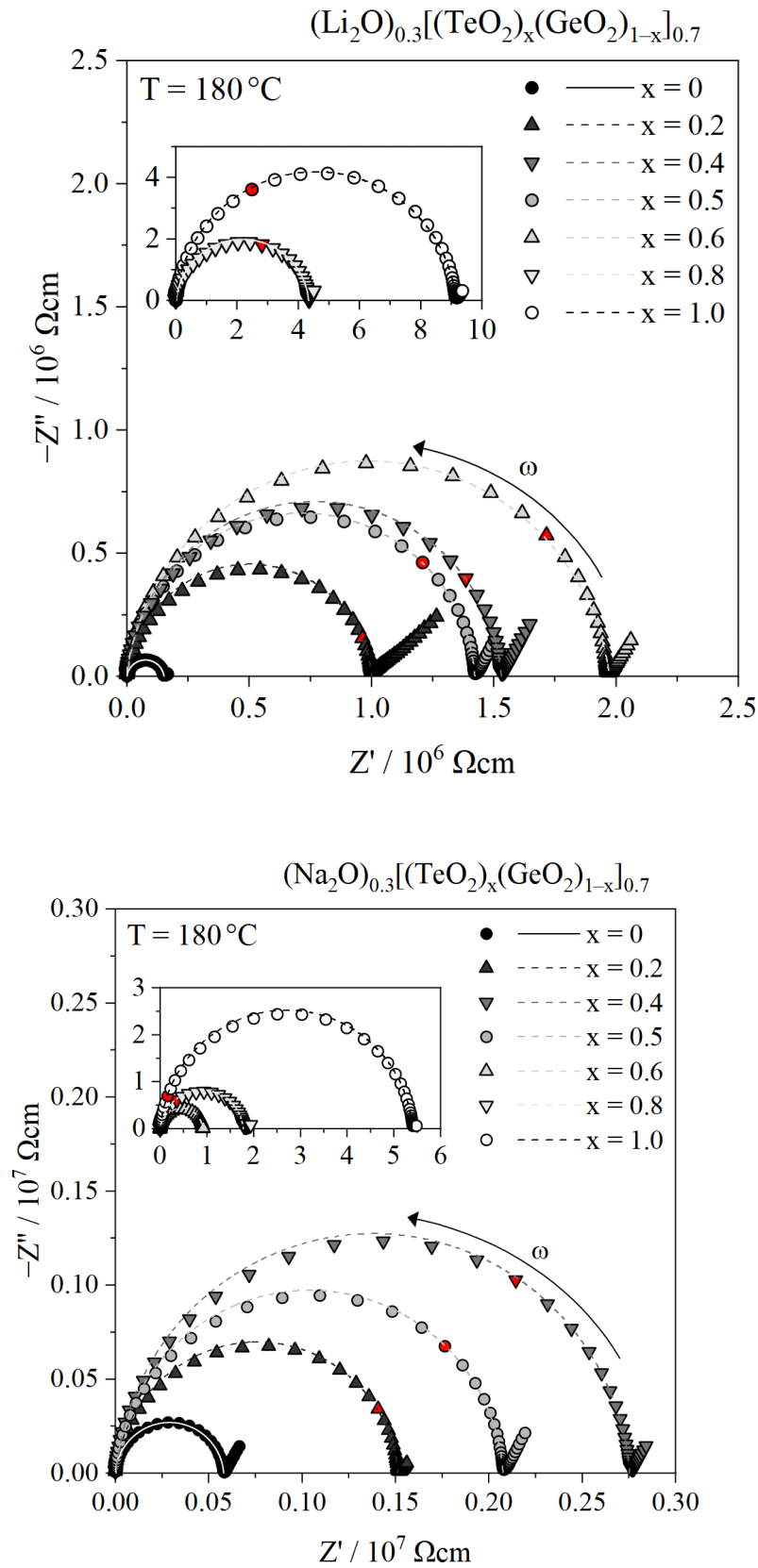


Figure S6: Complex plane plot of impedance data of $(\text{A}_2\text{O})_{0.3}[(\text{TeO}_2)_x(\text{GeO}_2)_{1-x}]_{0.7}$ ($\text{A} = \text{Li}, \text{Na}$) glasses recorded at 180 °C. Red data points indicate a frequency of 10 kHz. The solid and dashed lines indicate least-squares fits to the data according to the semi-circle function $y = -(y_0 + (r^2 - (x-x_0)^2)^{1/2})$, where x_0 and y_0 represent offsets on the Z' and Z'' axes respectively, and r represents the radius of the semi-circle. Data are divided by the geometrical factor l/S (l = sample thickness, S = area of the electrode), so the non-trivial zero of the fit function then corresponds to the real resistivity value, used to calculate the conductivity shown in the Arrhenius plots in Figure 1.

References

- [1] Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A., Rizzi, R., QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD, *J. Appl. Cryst.* 48 (2015). 598-603.
- [2] Grazulis, S., Chateigner, D., Downs, R. T., Yokochi, A. T., Quiros, M., Lutterotti, L., Manakova, E., Butkus, J., Moeck, P. & Le Bail, A., Crystallography Open Database – an open-access collection of crystal structures, *J. Appl. Cryst.* 42 (2009), 726-729.