Enhancing Electrical Conductivity and Catalytic Activity Through Controlled Crystallization of V_2O_5-Nb_2O_5-P_2O_5 Glass

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INTRODUCTION

- glassy and glass-ceramic materials based on V_2O_5-P_2O_5 have been identified as highly promising cathode materials for rechargeable Li-ion, Na-ion, and all-solid-state batteries
- these materials offer a compelling combination of high safety, exceptional energy density, and extended cycling life
- in addition, such materials are also recognized as effective catalysts in oxidation reactions
- thermally controlled crystallization of V_2O_5-P_2O_5-based glasses can significantly improve their microstructural properties, electrical conductivity, and electrochemical properties

RESEARCH AIM

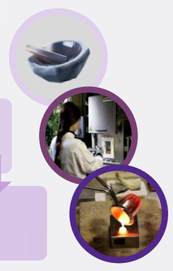
- the objective of this study is to synthesize a glass with a nominal composition of **$70V_2O_5$-$20Nb_2O_5$-$10P_2O_5$** and investigate the influence of controlled crystallization at different temperatures and durations on the electrical and catalytic properties

PREPARATION OF GLASS & GLASS-CERAMICS

1. Glass synthesis

Homogenization of starting mixture

Melting & Casting



70V-20Nb-10P glass (AS IS)

- black opaque glass

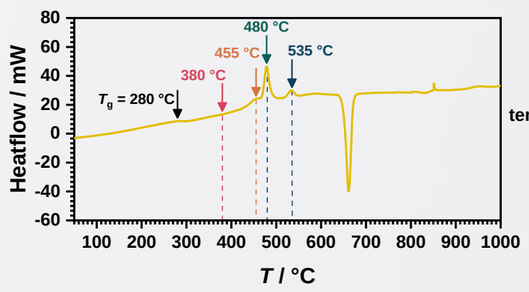
2. Glass-ceramic synthesis

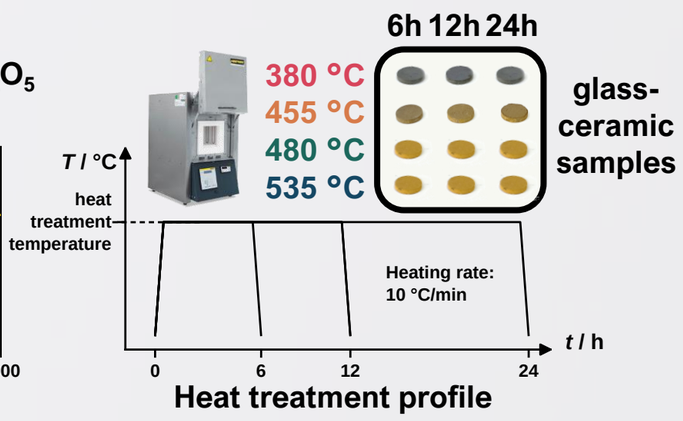
Crushing glass into powder

Pressing in order to form a pastille

Controlled crystallization

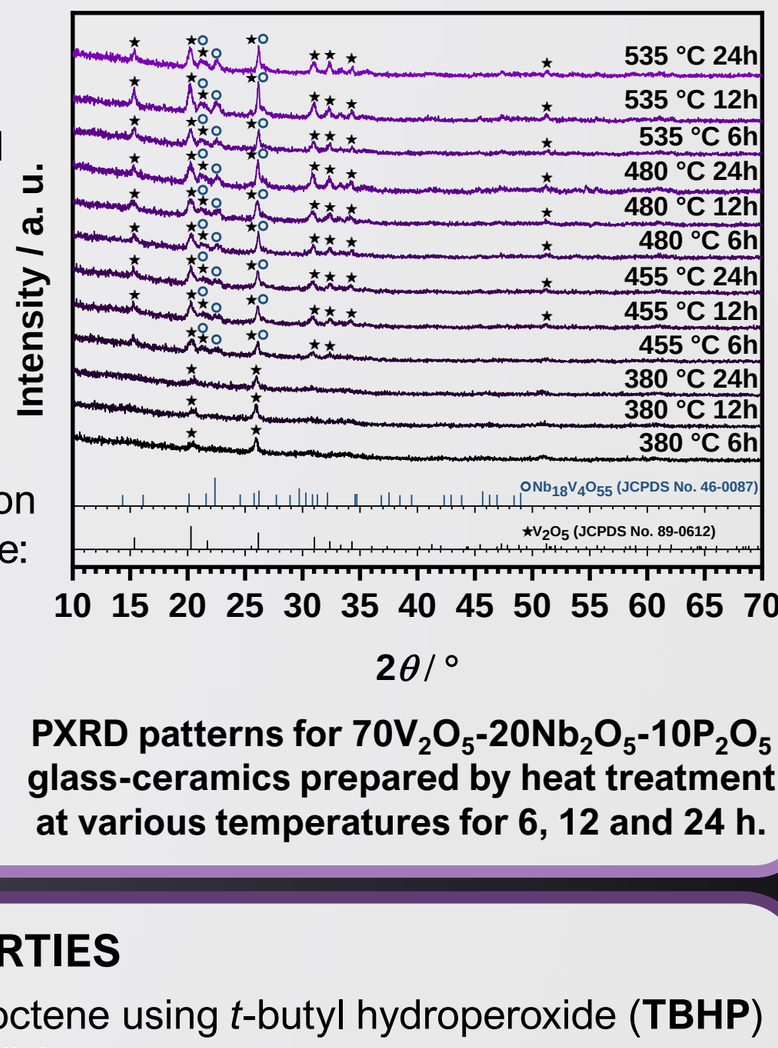
DTA curve of $70V_2O_5$-$20Nb_2O_5$-$10P_2O_5$ glass (AS IS)





PXRD ANALYSIS

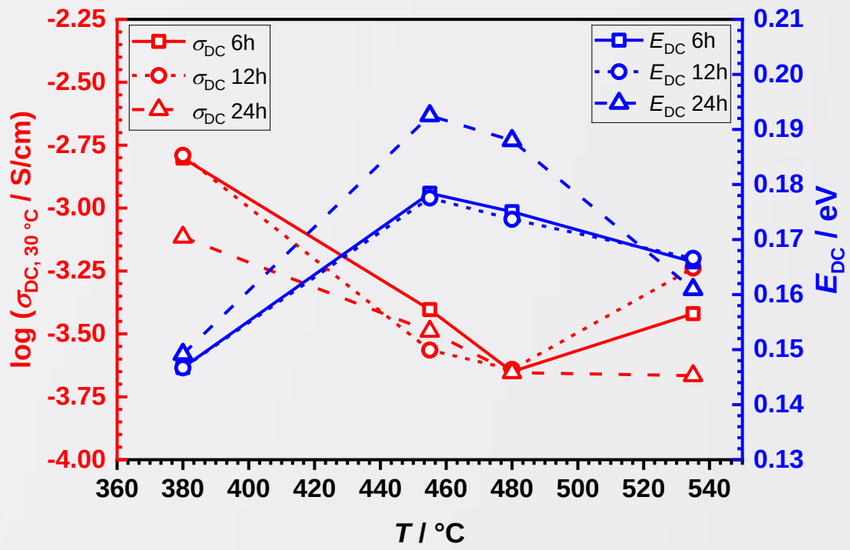
- PXRD patterns of samples heat-treated at 380 °C show only one crystal phase: **V_2O_5**
- heat-treatement above 380 °C results in the formation of an additional phase: **$Nb_{18}V_4O_{55}$**



PXRD patterns for $70V_2O_5$-$20Nb_2O_5$-$10P_2O_5$ glass-ceramics prepared by heat treatment at various temperatures for 6, 12 and 24 h.

ELECTRICAL PROPERTIES

- solid-state impedance spectroscopy (SS-IS)

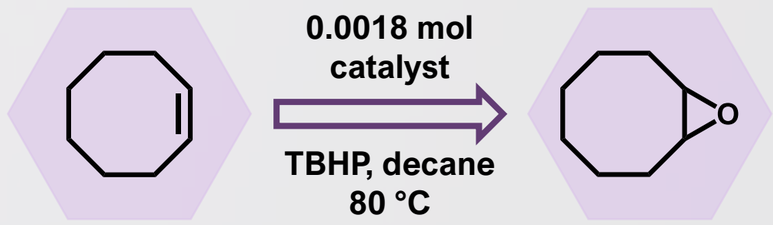


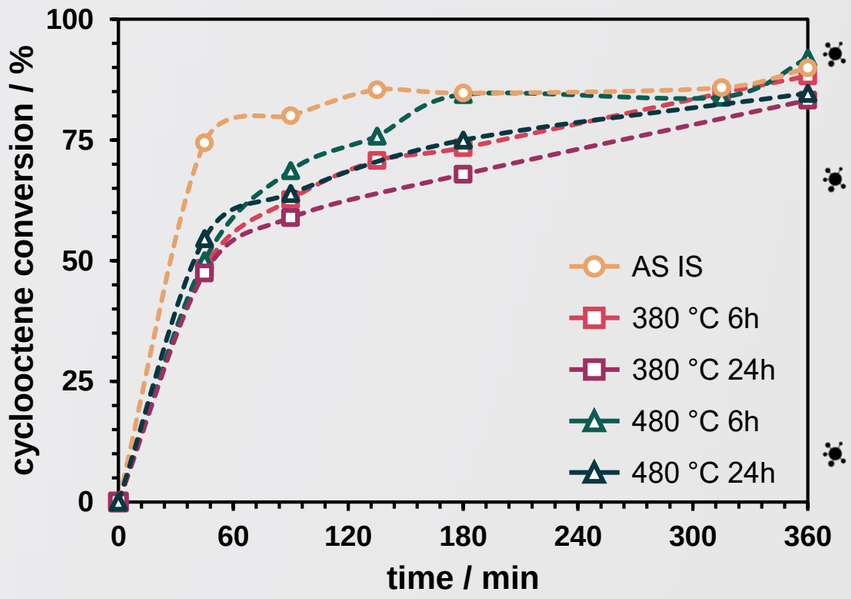
Compositional dependence of DC conductivity, σ_{DC}, at 30 °C and activation energy, E_{DC}

- sample heat-treated at 380 °C exhibits the highest conductivity of 1.58 mS/cm @30 °C

CATALYTIC PROPERTIES

- epoxidation of cyclooctene using *t*-butyl hydroperoxide (**TBHP**) in decane as the oxidizing agent





Converted cyclooctene vs. time with $70V_2O_5$-$20Nb_2O_5$-$10P_2O_5$ glass (AS IS) and selected glass-ceramic samples

- monitored by gas chromatography
- the non-treated sample (AS IS) shows the best catalytic activity: **90% conversion**
- the catalytic activity of the heat-treated samples slightly decreases compared to the non-treated sample

CONCLUSIONS

- ✓ 70V-20Nb-10P glass is successfully prepared and glass-ceramics are obtained by its controlled crystallization
- ✓ crystalline phases present in the prepared glass-ceramic samples are identified by PXRD
- ✓ samples heat-treated at 380 °C, which consist of only one crystal phase, **V_2O_5**, show the highest conductivity
- ✓ further heat treatment shows a negative effect on electrical conductivity, which could be a result of the appearance of an additional crystalline phase, **$Nb_{18}V_4O_{55}$**
- ✓ studied glass and glass-ceramics are highly active as catalysts in the epoxidation processes, with the non-treated sample exhibiting the highest catalytic activity

ASEC 2023 The 4th International Electronic Conference on Applied Sciences
27 October – 10 November 2023 | Online

This work is supported by the Croatian Science Foundation under the projects IP-2018-01-5425 and DOK-2021-02-9665.

This work is in part supported by COST Action NETPORE (CA20126), COST (European Cooperation in Science and Technology).