AusIMM

MOLTEN 2024

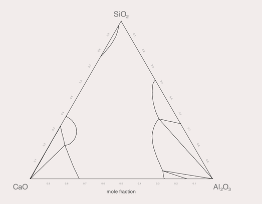
DECODING THE «GENOME» OF MOLTEN SLAGS BY MOLECULAR DYNAMICS SIMULATION

Mengyi Zhu, Jafar Safarian
Norwegian University of Science and Technology, Trondheim, Norway

MOTIVATION

How should we describe the features of slag melts? Does slag have a genome?

Current phase diagrams have no descriptions of the liquid slag region. However, a diagram for slag melt can guide us understand slag properties better.



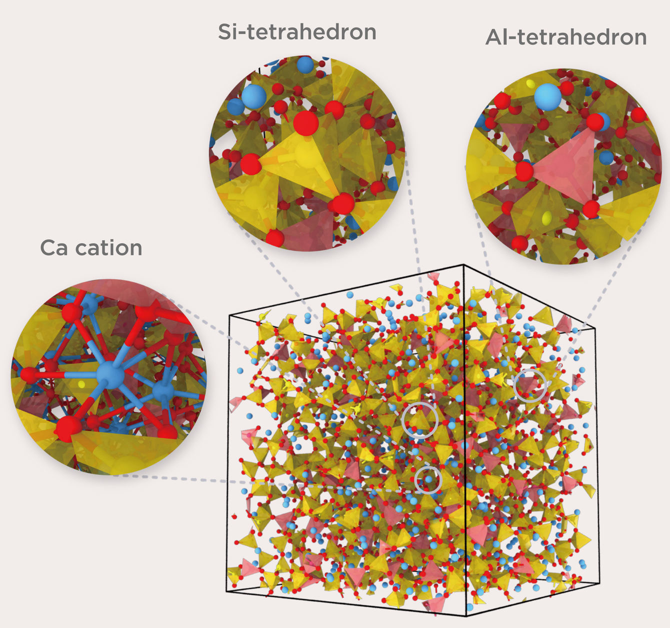
In this work, we utilize high-throughput MD simulations to study the $CaO-Al_2O_3-SiO_2$ slag system. A slag predominant oxygen species diagram was established based on identified oxygen-centric slag gene units. It is also proposed to extend the oxygen classification to better reflect the features of the Al_2O_3-bearing slag system, where the charge compensation effect plays a crucial role.

METHODS

1. Evenly divide the entire $CaO-Al_2O_3-SiO_2$ slag system into 231 slag composition points at 5 mol% intervals.
2. High-throughput MD simulations performed using LAMMPS software with the Jakse potential.
   All slag samples initially relaxed at 4000 K followed by cooling to 2073 K. NPT, NVT, and NVE ensembles included to achieve the final slag structures.
3. Data collection and post-processing for slag structural analysis using Python.

Scan for slag safari

Click to start



CONCLUSION

This study highlights the importance of medium-range order of slag melts. Different oxygen species in the $CaO-Al_2O_3-SiO_2$ ternary system were detected. A predominant oxygen species diagram was established for the first time. Furthermore, the conventional oxygen classification is proposed to be extended to better adapt to the charge compensation effect of Al_2O_3.

REFERENCES

Bouhadja, M., Jakse, N., & Pasturel, A. (2013). The Journal of chemical physics, 138(22).
Zhu, M., Wu, G., Tang, K., Müller, M., & Safarian, J. (2024). Chemical Engineering Journal, 488, 150788.
Zhu, M., Wu, G., Azarov, A., Monakhov, E., Tang, K., Müller, M., & Safarian, J. (2021). MMTB, 52(5), 3045-3063.

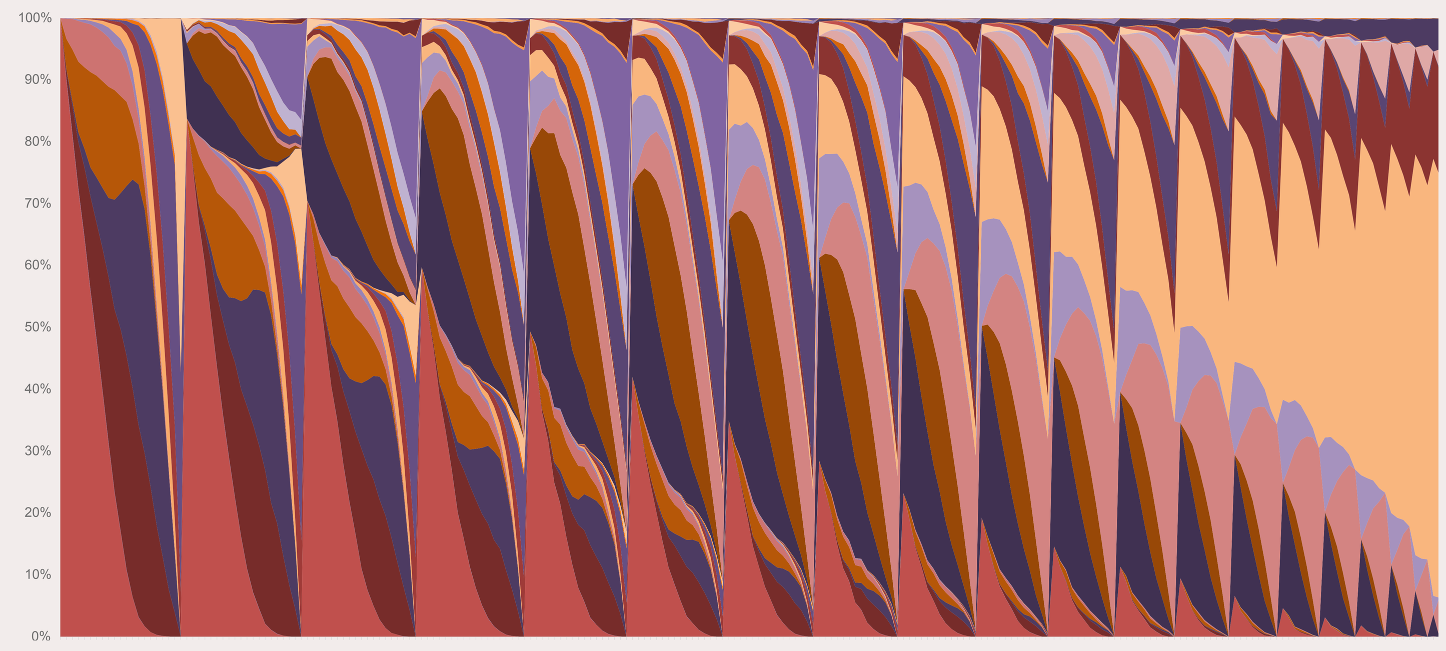
RESULTS AND DISCUSSIONS

OVERVIEW OF 231 SLAGS

60 different oxygen micro-environments detected in total

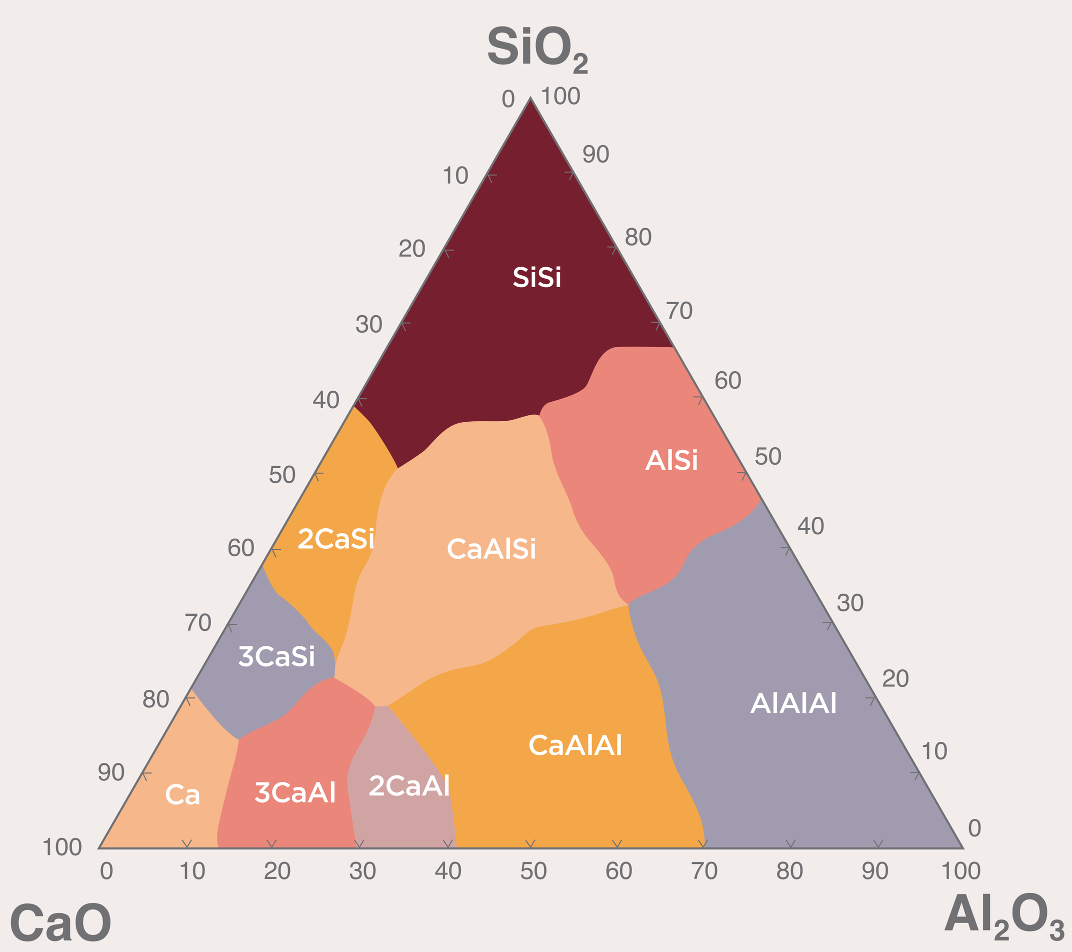
21 with contents exceeding 5% at least once

10 identified as the most abundant species

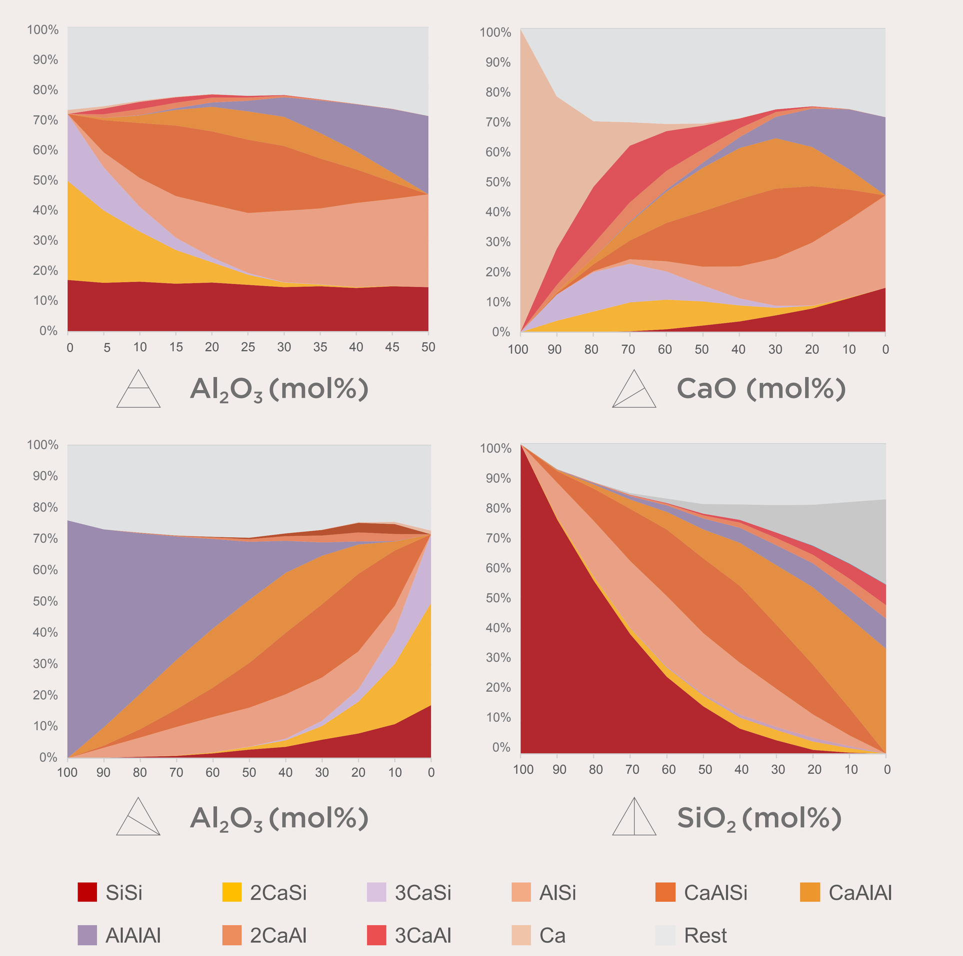


Distribution of different oxygen micro-environments obtained from MD simulation of 231 slags. The far left represents the $CaO-SiO_2$ binary system, with Al_2O_3 molar fraction increasing by 5 mol% steps to the far right, unary Al_2O_3.

PREDOMINANT OXYGEN SPECIES DIAGRAM



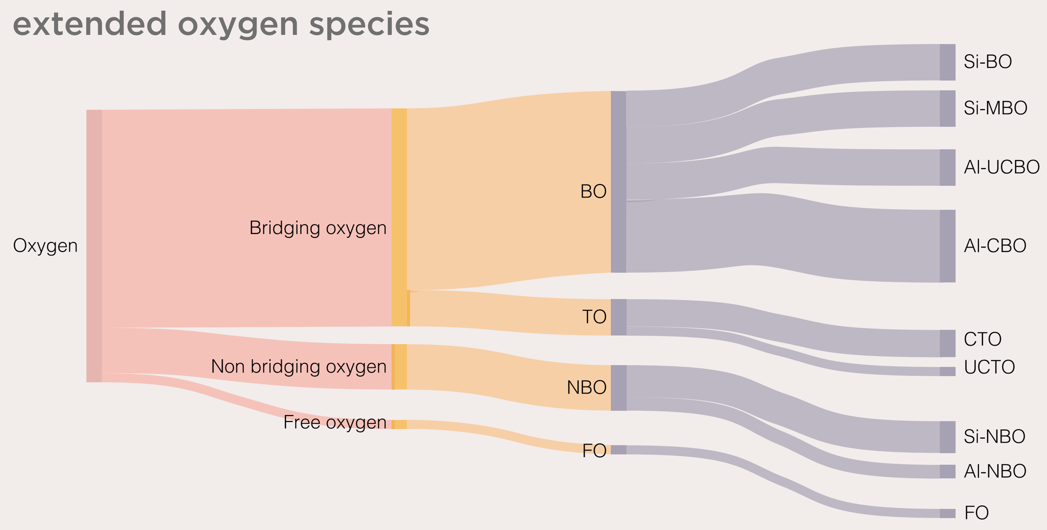
Established predominant oxygen species diagram



Oxygen species content along specific composition lines

EXTENDED OXYGEN CLASSIFICATION

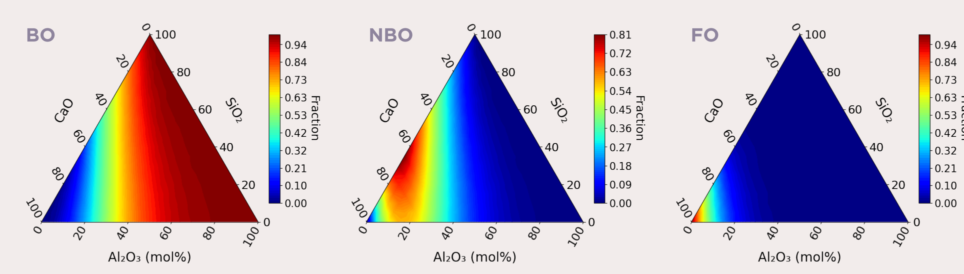
Relationship between conventional and extended oxygen species



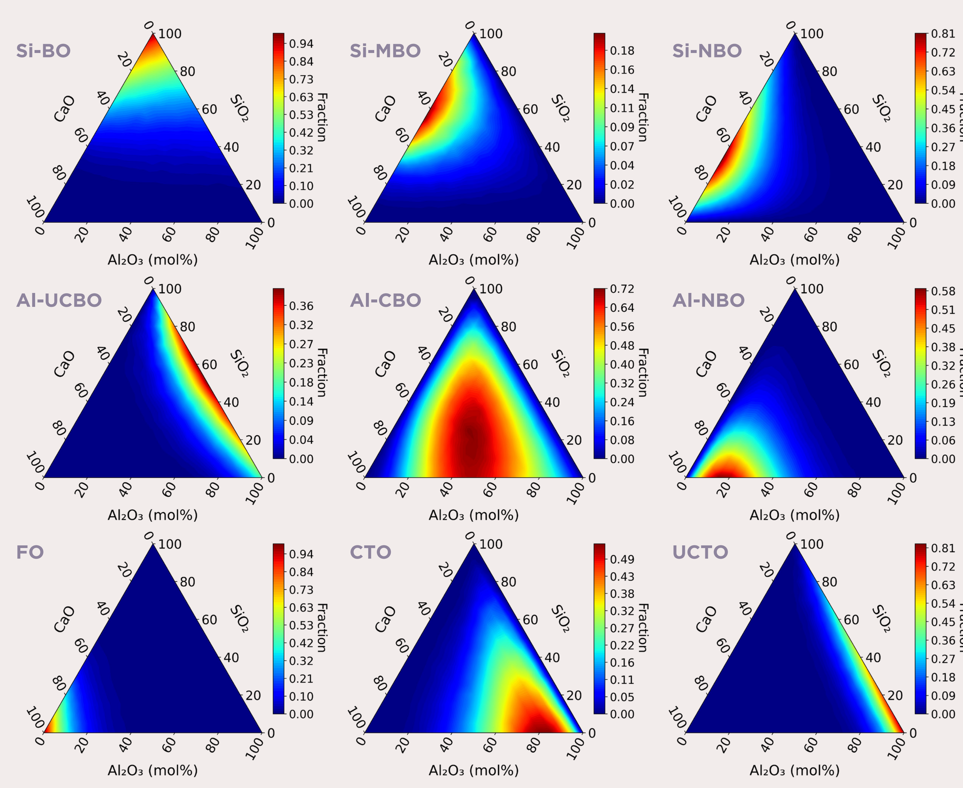
Nomenclature and definition of extended oxygen species

NOMENCLATURE	DEFINITION
Si-BO	Oxygen only coordinated with two Si-tetrahedra
Si-MBO	Oxygen coordinated with two Si-tetrahedra and with adjacent modifier
Al-UCBO	Oxygen coordinated without compensated Al-tetrahedron
Al-CBO	Oxygen coordinated with compensated Al-tetrahedron
CTO	Tricluster oxygen with compensated Al-tetrahedron
UCTO	Tricluster oxygen without compensated Al-tetrahedron
Si-NBO	NBO bonded with Si
Al-NBO	NBO bonded with Al
FO	Free oxygen

Conventional oxygen types:



Extended oxygen types:



Distriution of different extended oxygen species

Mengyi Zhu
Postdoc researcher at NTNU, Norway
Conference Day 2 - Session 20 - Physicochem. Pros.
mengyi.zhu@ntnu.no
Tel: +47 45885932

SisAl Pilot NTNU