Supporting Information

Elucidating the role of intrinsic defects on dosimetric properties of the MgB_4O_7 compound: an atomistic simulation approach

Raíssa Contassot,[a] João Batista,[a] André Otsuka,[b] Antônio Souza,[c] Edward Ferraz,[c] Adelmo Souza,[d] Jorge L. O. Santos,[d] Vinicius Coelho[d] and Heveson Lima[e]

[a]Departamento de Ciências Exatas e Sociais Aplicadas, Universidade Federal de Ciências da Saúde de Porto Alegre, 40050-170, Porto Alegre, RS, Brazil

[b]Departamento de Física, Universidade Federal de Sergipe, 49100-000, São Cristóvão, SE, Brazil

[c]Centro das Ciências Exatas e das Tecnologias, Universidade Federal do Oeste da Bahia, 47808-021, Barreiras, BA, Brazil

[d]Centro Multidisciplinar de Bom Jesus da Lapa, Universidade Federal do Oeste da Bahia, 47600-000, Bom Jesus da Lapa, BA, Brazil

[e]Centro Multidisciplinar de Luís Eduardo Magalhães, Universidade Federal do Oeste da Bahia, 47850-000, Luís Eduardo Magalhães, BA, Brazil

(A) Oxide precursors (MgO and B_2O_3)

Table S1- Lattice parameters for MgO.

Lattice parameters	Ref. [1]	This work	%
a (Å)	4.217	4.275	1.37
V (Å^3)	74.991	78.107	4.15

Table S2- Elastic constants (in GPa) for MgO.

Elastic constants	Ref. [2]	This work	%
C_{11}	297.00	267.91	-9.80
C_{12}	95.20	118.16	24.11
C_{44}	155.70	190.61	22.42

For MgO, BSM potential was used to remove the Cauchy violation in the elastic constants: r_0=0.221 Å and K= 134.546 eVÅ^{-2}.

Table S3- Dielectric constants for MgO.

Dielectric constants	Ref. [3]	This work	%
e_0	9.90	11.57	16.87
e_∞	-	3.02	-

Table S4- Lattice parameters for trigonal B_2O_3.

Lattice parameters	Ref. [4]	This work	%
a(Å)	4.335	4.302	-0.76
c(Å)	8.341	8.245	-1.16
V(Å^3)	135.759	132.142	-2.66

Table S5- Elastic constants (in GPa) for trigonal B_2O_3.

Elastic Constants	Ref. [5]	This work	%
C_{11}	223.4	230.930	3.37
C_{12}	58.9	70.375	19.48
C_{13}	-	11.701	-
C_{14}	-	10.904	-
C_{33}	-	72.537	-
C_{44}	-	47.333	-
C_{66}	-	80.277	-

We have used the results obtained with the B1 potential of Takada's work [5] for sake of comparison. There, just C_{11} and C_{12} are shown.

Table S6- Dielectric constants for trigonal B_2O_3.

Dielectric constants	Ref. [6]	This work	%
e_0	3.98	4.86	22.11
e_∞	-	2.96	-

(B) Defect calculations

Table S7- Lattice energy for orthorhombic MgB_4O_7 and oxide precursors.

Materials	Lattice energies (eV)
MgB_4O_7	-466.399
MgO	-38.785
B_2O_3	-209.248

Table S8-Defect formation energy for isolated defects.

Defect Energy (eV)				
$V_B^{'''}$	$V_{Mg}^{''}$	$V_O^{\bullet\bullet}$	$Mg_B^{'}$	$B_{Mg}^{\bullet}$
82.455	24.051	31.586	52.730	-35.965

Interstitial Position	B_i	Mg_i	O_i
(4/5,3/5,9/10)	-60.716	-15.641	-
(3/10,3/10,1/10)	-	-15.641	-
(4/5,3/10,1/3)	-	-14.804	-23.314
(1/5,7/10,3/5)	-49.031	-15.641	-10.434

Table S9-Solution energies for intrinsic defects, normalized per defect.

Defect type	Solution energy (eV/def)
Mg Frenkel	4.2048
B Frenkel	11.3695
O Frenkel	4.1363
MgB_4O_7 Schottky	9.3814
MgO Schottky	8.4262
B_2O_3 Schottky	10.4842
MgB_4O_7 anti-Schottky	3.7248
MgO anti-Schottky	-0.0851
B_2O_3 anti-Schottky	3.5749
Mg_B antisite	6.0059

Reference

1 S. Sasaki, K. Fujino and Y. Takéuchi, *Proc. Japan Acad. Ser. B*, 1979, **55**, 43–48.

2 C.-S. Zha, H.-K. Mao and R. J. Hemley, *Proc. Natl. Acad. Sci.*, 2000, **97**, 13494–13499.

3 M. A. Subramanian, R. D. Shannon, B. H. T. Chai, M. M. Abraham and M. C. Wintersgill, *Phys. Chem. Miner.*, 1989, **16**, 741–746.

4 M. Burianek, J. Birkenstock, P. Mair, V. Kahlenberg, O. Medenbach, R. D. Shannon and R. X. Fischer, *Phys. Chem. Miner.*, 2016, **43**, 527–534.

5 A. Takada, C. R. A. Catlow and G. D. Price, *J. Phys. Condens. Matter*, 1995, **7**, 8659–8692.

6 L. Li, W. Bin Hong, X. J. Yan and X. M. Chen, *Int. J. Appl. Ceram. Technol.*, 2019, **16**, 2047–2052.