

Phase diagram of GaN

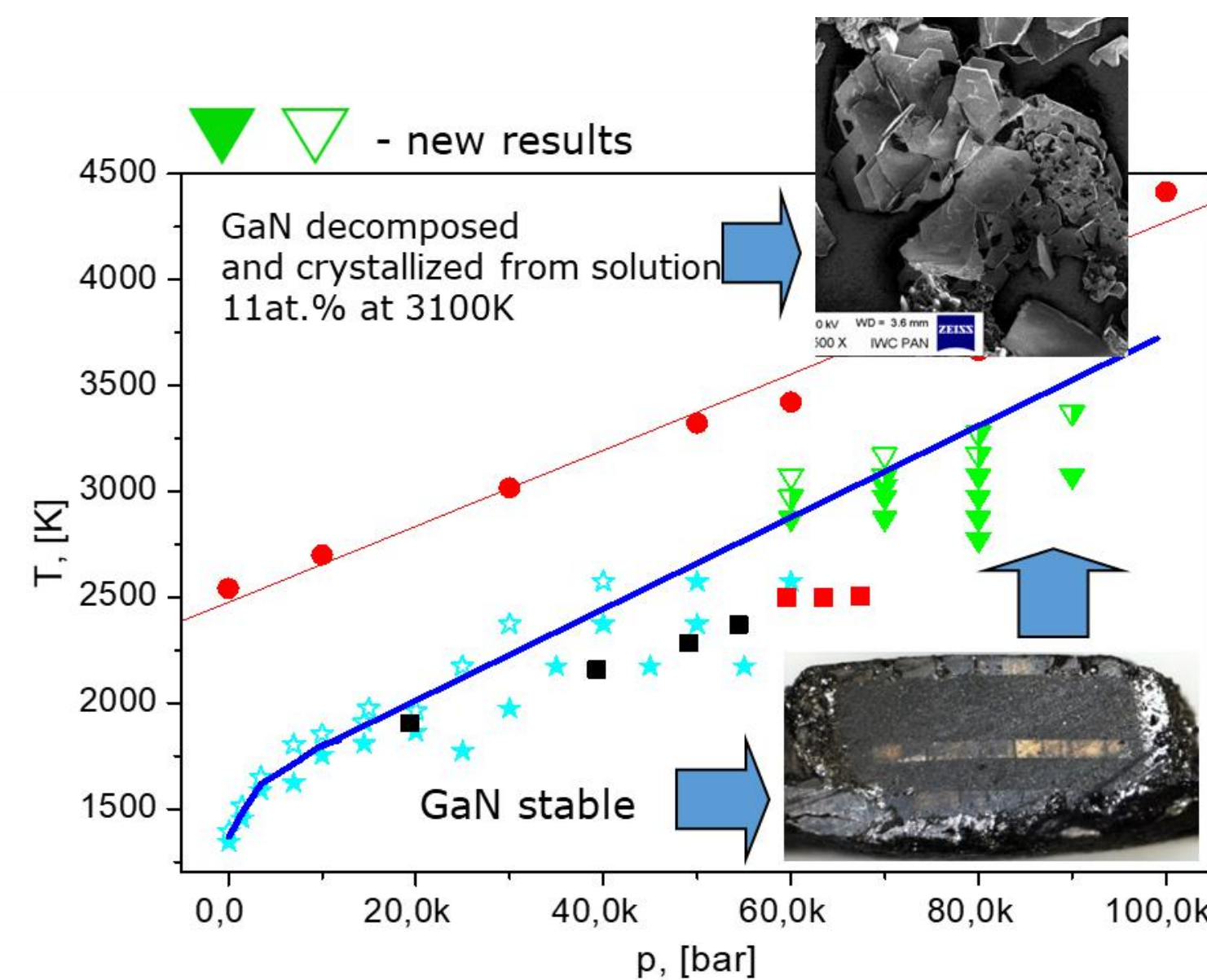
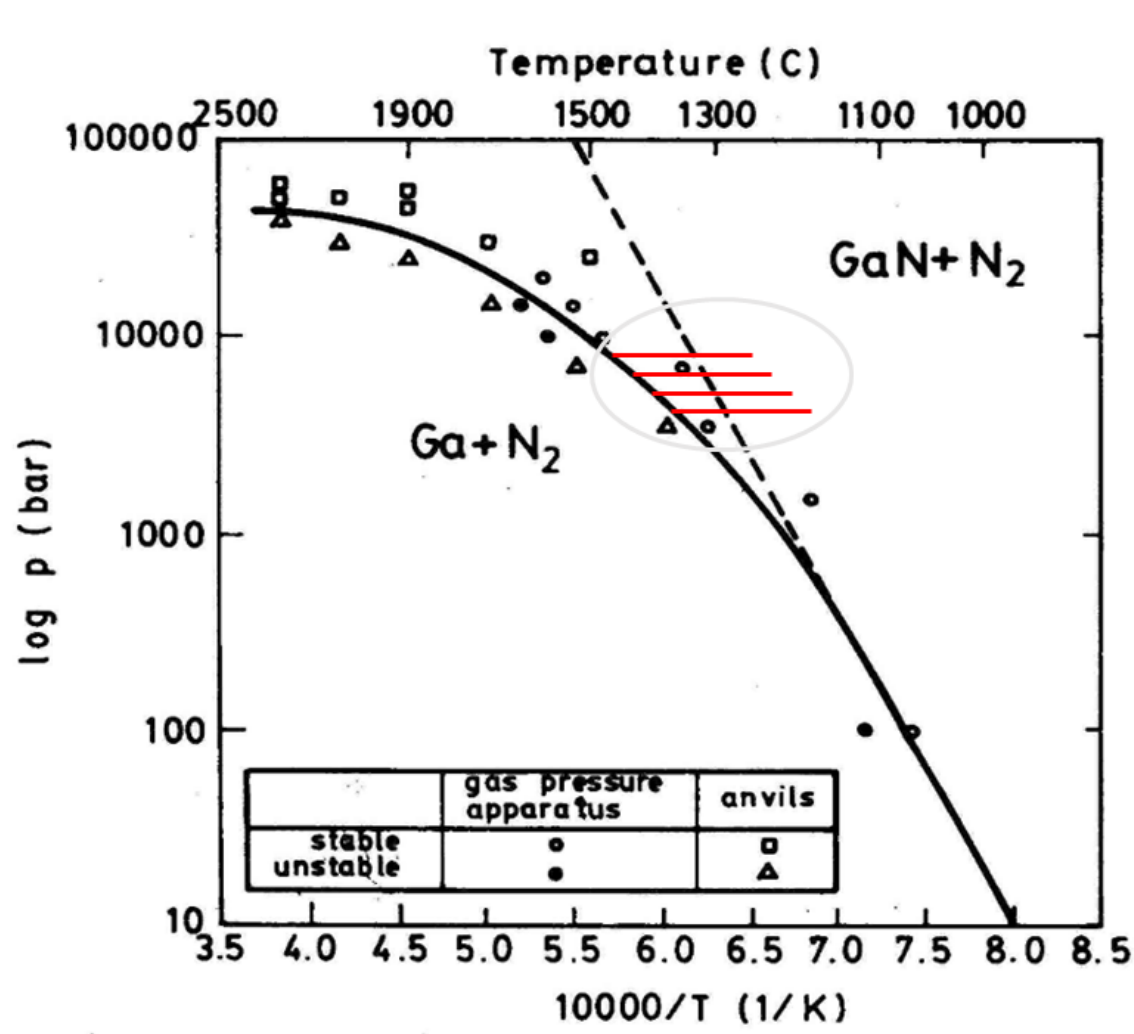
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Abstract

Physics and technology of GaN are very much advanced due to excellent figures of merit relevant for important applications. Nevertheless the GaN phase diagram, including the melting curve, has not been fully determined. Below both experimental and theoretical research in this area conducted at Unipress is summarized. In particular, an excellent agreement of the recent simulation results by *ab initio* Molecular Dynamics with well-established experimental data on GaN decomposition is shown.

Thermal stability of GaN

GaN decomposes at high temperatures, and to suppress this process, a high pressure of nitrogen is necessary. The famous equilibrium curve for GaN and its constituents was first published in 1984 [1] and, extended up to 9 GPa and corresponding temperatures exceeding 3000 K [2].

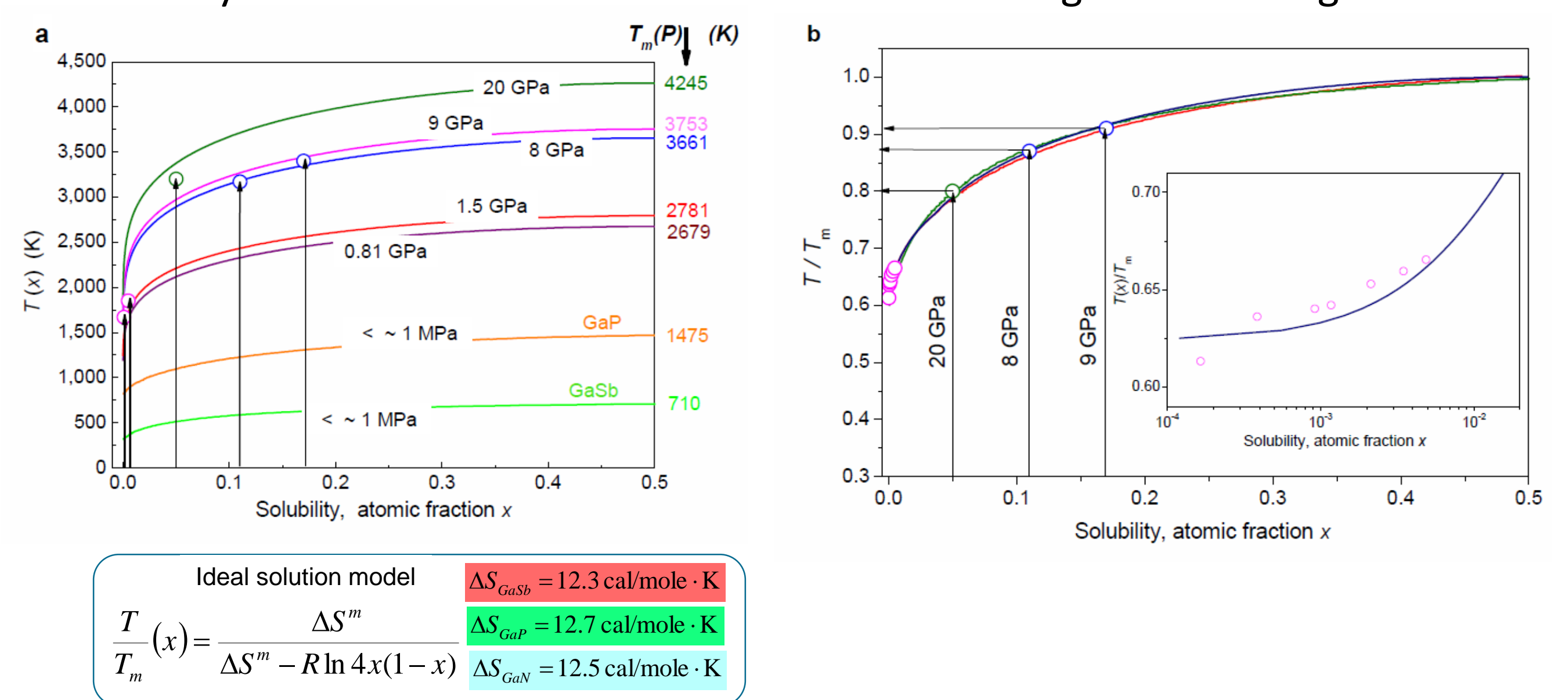


J. Karpiński, J. Jun and S. Porowski, J. Cryst. Growth 66, 1, p., 1984

S. Porowski et al. J. of Physics and Chemistry of Solids 85, 2015

Solubility and melting curve of GaN

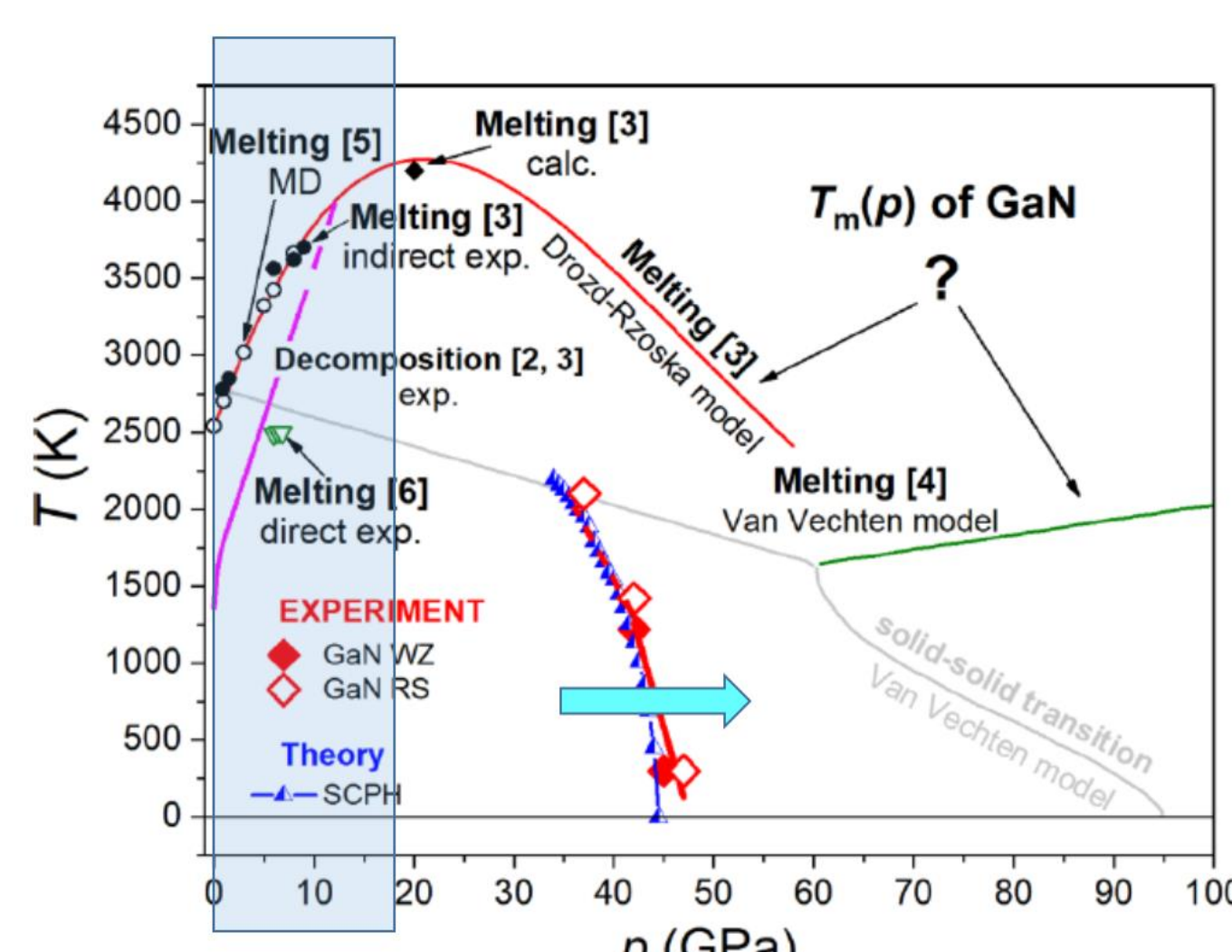
The solubility data, even at temperature as high as > 3000 K, clearly indicated that the system was still far from conditions of the congruent melting of GaN.



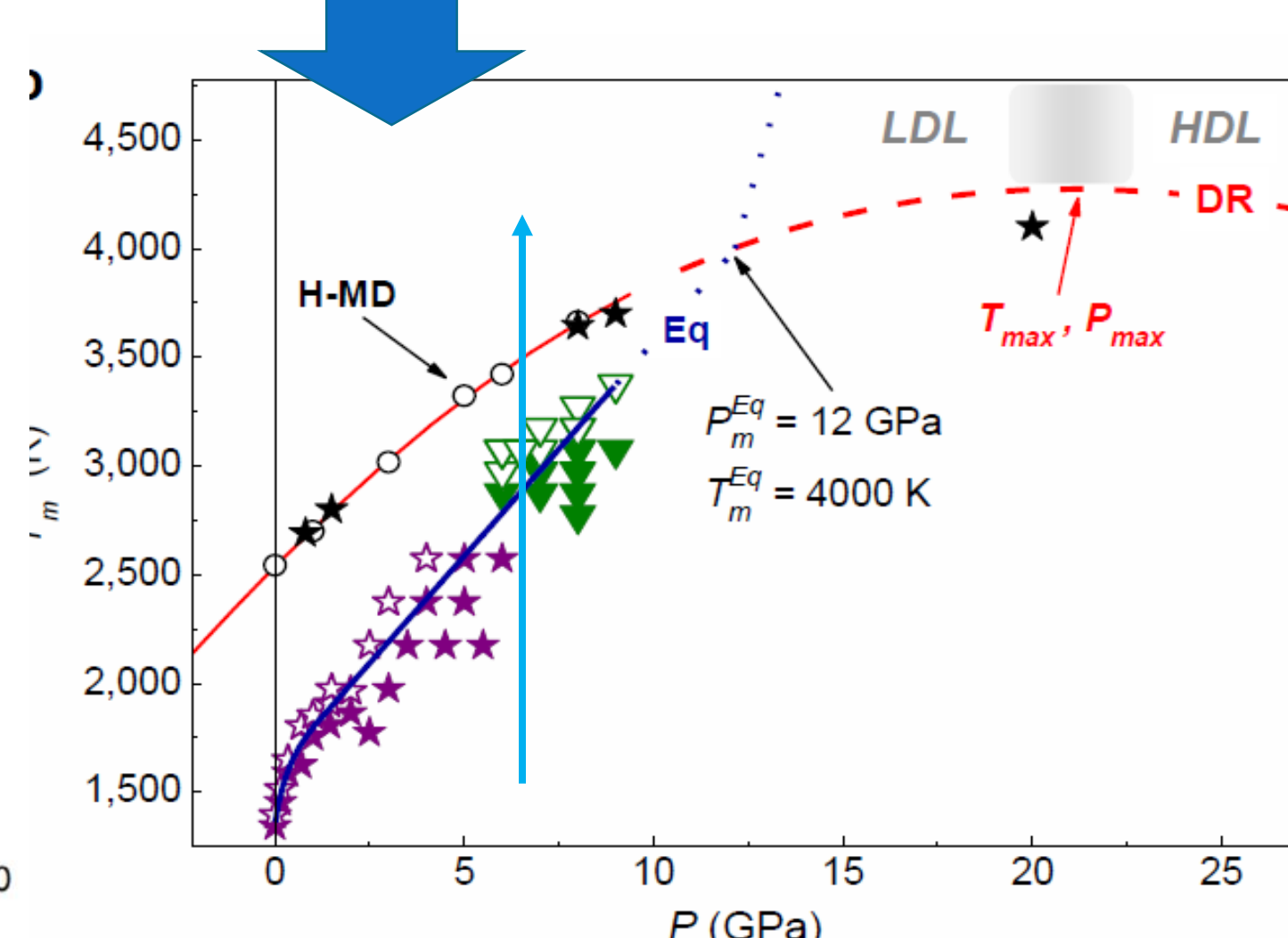
From the solubility data, the melting temperature in function of pressure has been evaluated and the resulting dependence was in a very good agreement with a conventional MD studies by Harafuji et al. [3] although in disagreement with Van Vechten model [4] and some experimental suggestions [5].

Decomposition and melting of GaN - EXPERIMENT

We think that the decomposition curve and the melting curve look like this meaning that at low pressures (< 12 GPa), at heating, GaN decomposes before melting.



Current state of p-T phase diagram of GaN as published in [6]. The „Low pressure” part is shadowed.

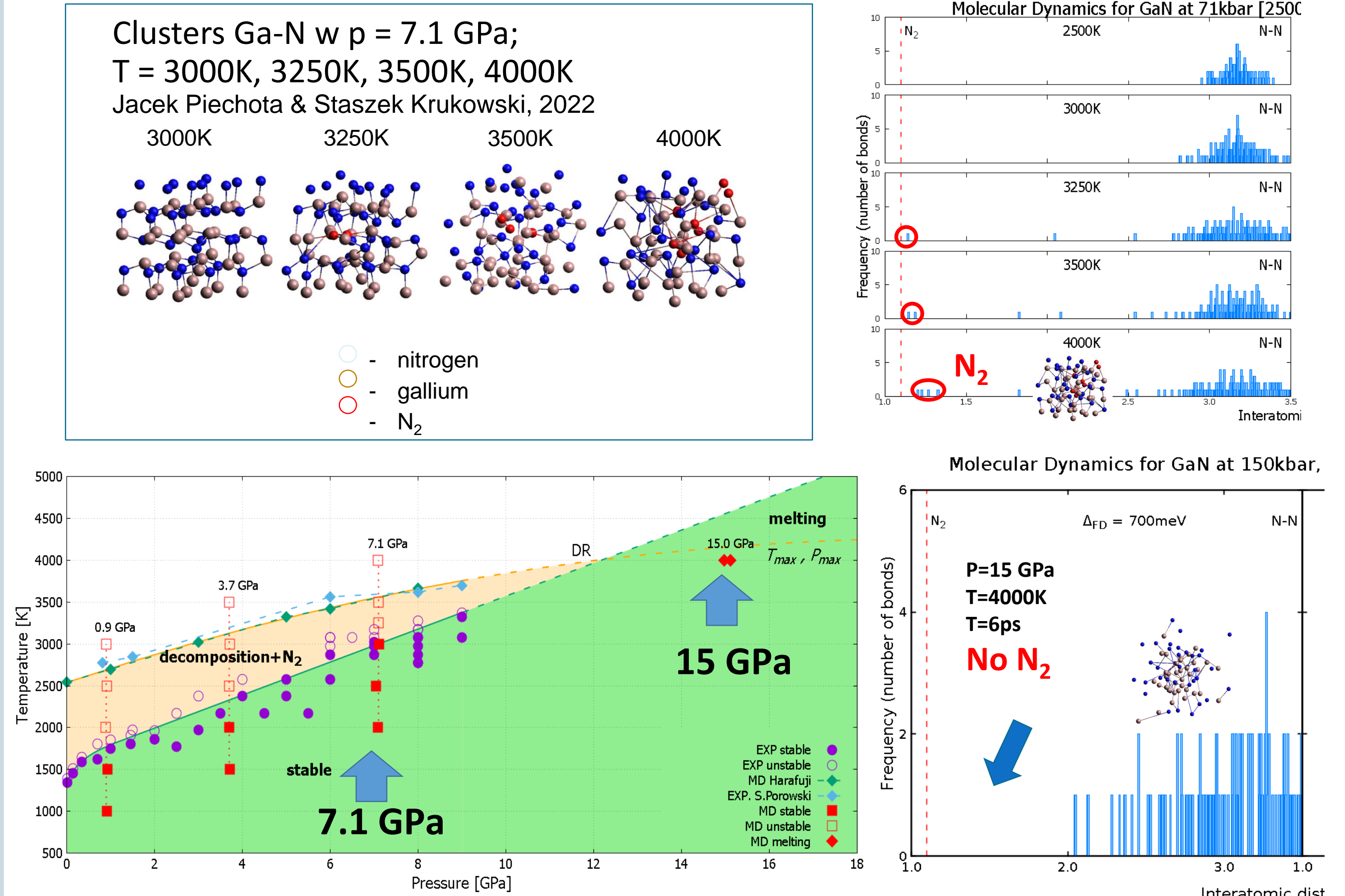


The „Low pressure” part of the p-T phase diagram following from [1,2,3] and confirmed by *ab initio* MD

References

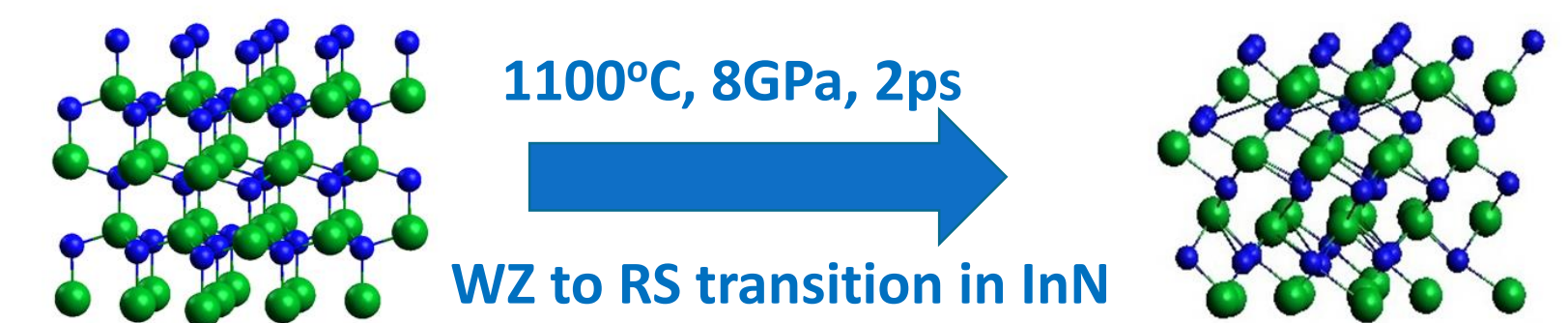
1. J. Karpiński, J. Jun, S. Porowski, J Cryst Growth, 66, 1-10, 1984
2. S. Porowski, B. Sadovyi, S. Gierlotka, S.J. Rzoska, I. Grzegory, I. Petruscha, V. Turkevich, D. Stratiichuk, Journal of Physics and Chemistry of Solids, 85, 138-143, 2015
3. K. Harafuji, T. Tsuchiya, and K. Kawamura, J. Appl Phys. 96, 2501, 2004)
4. J. A. Van Vechten, Phys. Rev. B 7, 1479, 1973
5. W. Utsumi, H. Saitoh, H. Kaneko, T. Watanuki, K. Aoki, and O. Shimomura, Nature Materials 2, 735, 2003
6. B. Sadovyi, M. Wierzbowska, S. Stelmakh, S. Boccatto, S. Gierlotka, T. Irifune, S. Porowski and I. Grzegory, Phys. Rev. B 102, 235109, 2020

Decomposition vs melting of GaN - Ab initio MD



Conclusion and outlook

1. The *ab initio* MD results are in good agreement with experimental data of [1,2] and with conventional MD data of [3]
2. Continuation:
 - *ab initio* MD of GaN in rocksalt phase
 - Experiment: GaN melting by XRD in LH DAC
 - *ab initio* MD of InN



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