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МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ТЕПЛОФИЗИЧЕСКИХ СВОЙСТВ МЕТАНА ПРИ СТАТИЧЕСКОМ И УДАРНО-ВОЛНОВОМ СЖАТИИ*

А. В. Кудинов[1], Ю. А. Богданова[2], С. А. Губин[3], З. И. Мамедов[4]

Аннотация: Методом молекулярной динамики (МД) проведено моделирование термодинамических характеристик жидкого метана при изотермическом сжатии. Расчеты проведены с помощью пакета молекулярно-динамического моделирования LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), в котором реализована поддержка реакционного силового поля ReaxFF. Моделирование ударно-волнового сжатия жидкого метана проведено методом Гюгониостата в диапазоне давлений 1000–44 000 атм. Аналогичные расчеты выполнены на основе теоретически обоснованного уравнения состояния плотного газа с использованием потенциала межмолекулярного взаимодействия Exp-6. Получены зависимости давления на изотерме и ударной адиабате от степени сжатия жидкого метана, а также зависимости скорости ударной волны от массовой скорости. Результаты расчетов согласуются с экспериментальными данными.

Ключевые слова: молекулярно-динамическое моделирование; изотермическое сжатие; ударная адиабата; метан

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[1]Национальный исследовательский ядерный университет «МИФИ», swen379@gmail.com
[2]Национальный исследовательский ядерный университет «МИФИ», bogdanova.youlia@bk.ru
[3]Национальный исследовательский ядерный университет «МИФИ», gubin_sa@mail.ru
[4]Национальный исследовательский ядерный университет «МИФИ», ZaurMam@inbox.ru

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MOLECULAR DYNAMIC SIMULATION OF ISOTHERMAL AND SHOCK-INDUCED COMPRESSION OF METHANE

A. V. Kudinov, Yu. A. Bogdanova, S. A. Gubin, and Z. I. Mamedov

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation

Keywords: A molecular dynamic (MD) simulation of isothermal compression of liquid methane ($T = 110$ K) using LAMMPS code and ReaxFF potential is performed. The influence of Nosé–Hoover thermostat and barostat on thermodynamic properties is analyzed. Isothermal curves for $T = 110$ K and $P = 50$–1800 atm were simulated. Hugoniostat simulation was conducted for pressures $P = 1000$–$44\,000$ atm. For the same interval of pressures, a simulation using Exp-6 potential was carried out. A Hugoniot curve for liquid methane and a dependence of shock wave velocity on the particle velocity were obtained. The MD simulation provides very good estimates for the thermodynamic properties of methane when applied to the isothermal and shock-induced compression.

Keywords: molecular dynamic simulation; isothermal compression; shock Hugoniot, methane

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Contributors

Kudinov Andrey V. (b. 1996) — student, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; swen379@gmail.com

Bogdanova Youlia A. (b. 1983) — assistant, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; bogdanova.youlia@bk.ru

Gubin Sergey A. (b. 1945) — Doctor of Science in physics and mathematics, professor, Head of Department, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; gubin_sa@mail.ru

Mamedov Zaur Ilgam Ogly (b. 1997) — student, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; ZaurMam@inbox.ru