Hydrogen Storage: Simulations on $LaNi_5H_6$

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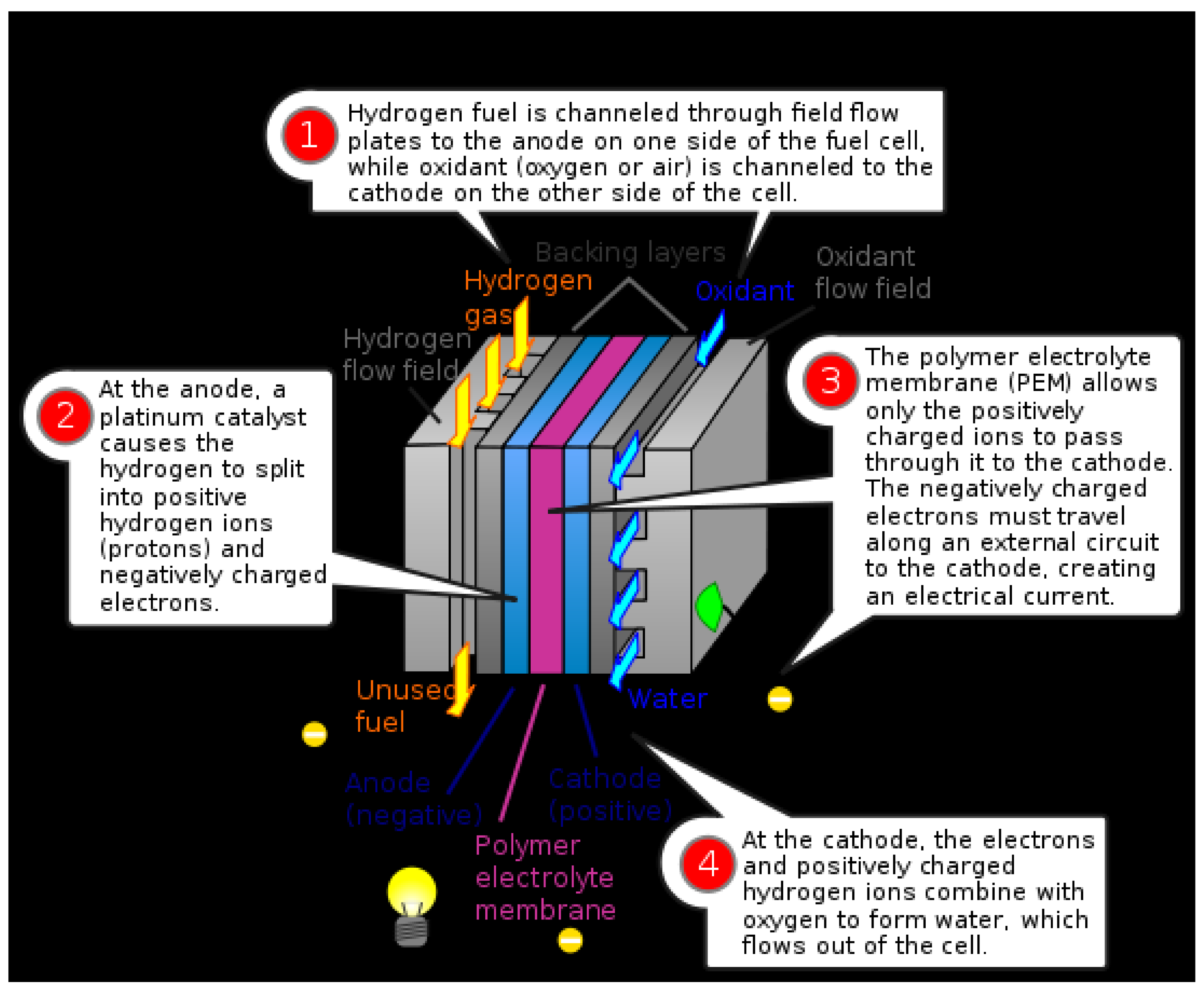
Abstract

It was the goal of the research conducted this summer to investigate an efficient way of storing hydrogen in a metal alloy of lanthanum and nickel ($LaNi_5$). A series of Monte Carlo simulations were performed, utilizing a Grand Canonical code, in order to accomplish this. Throughout the course of the research it was important to first obtain a useable potential energy function (usually referred to as a force field). Once accomplished, the next step was to begin optimizing certain conditions under which the simulations were taking place. Among other things, the temperature of the system was varied (attempting to stay close to room temperature, as it is easy to achieve), as well as pressure (the closer to atmospheric pressure, the safer), and weight of the metal alloy (keeping in mind that the lighter the system, the easier it is to transport.

Introduction



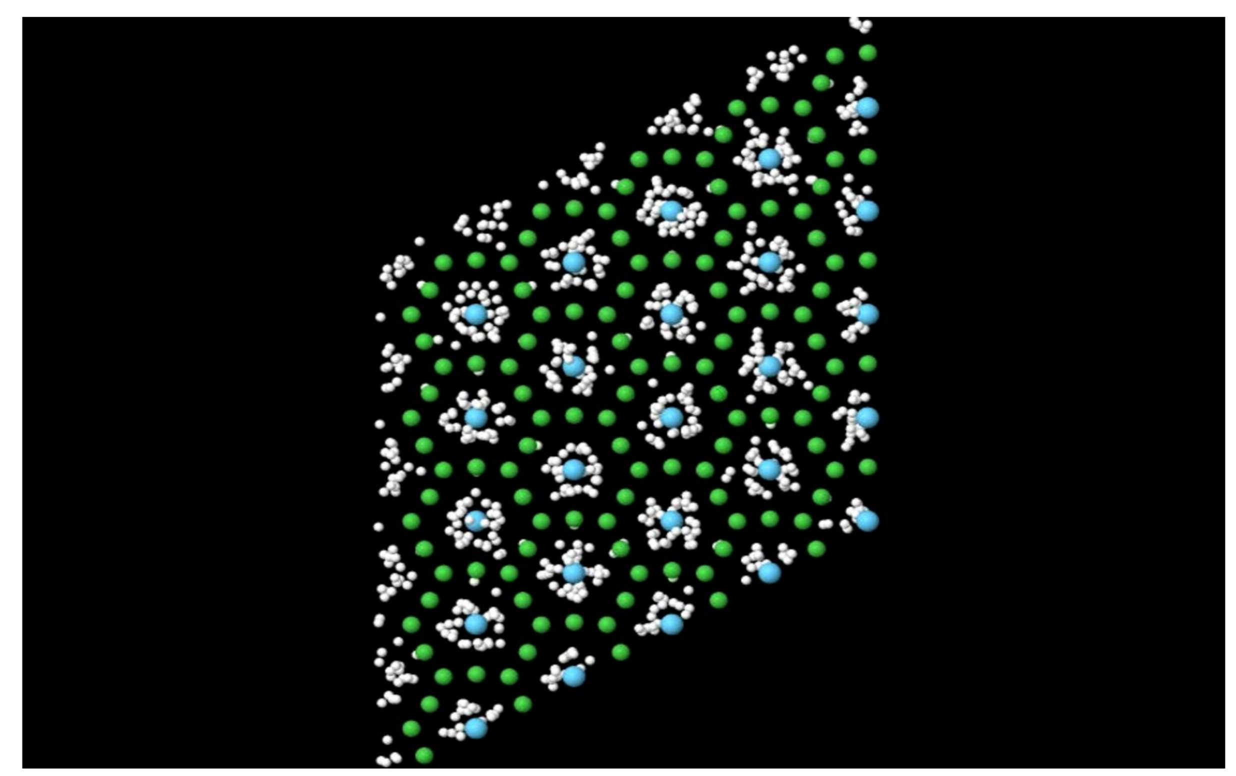
There has been a recent effort to move from fossil fuels and hydrocarbons to a cleaner source of energy. Using hydrogen as a source of energy accomplishes just this – whether it is used for combustion or to power a fuel cell, the only product is water. The main barrier standing in the way of realizing this transition is the current inability to store quantifiable (large) amounts of hydrogen in mobile vessels. In addition to being mobile (small and light enough to transport), the containers must be safe for practical use (i.e. they must be amenable to atmospheric temperature and pressure). If this problem can be solved, then the use of hydrogen as a fuel source can suddenly become a reality.

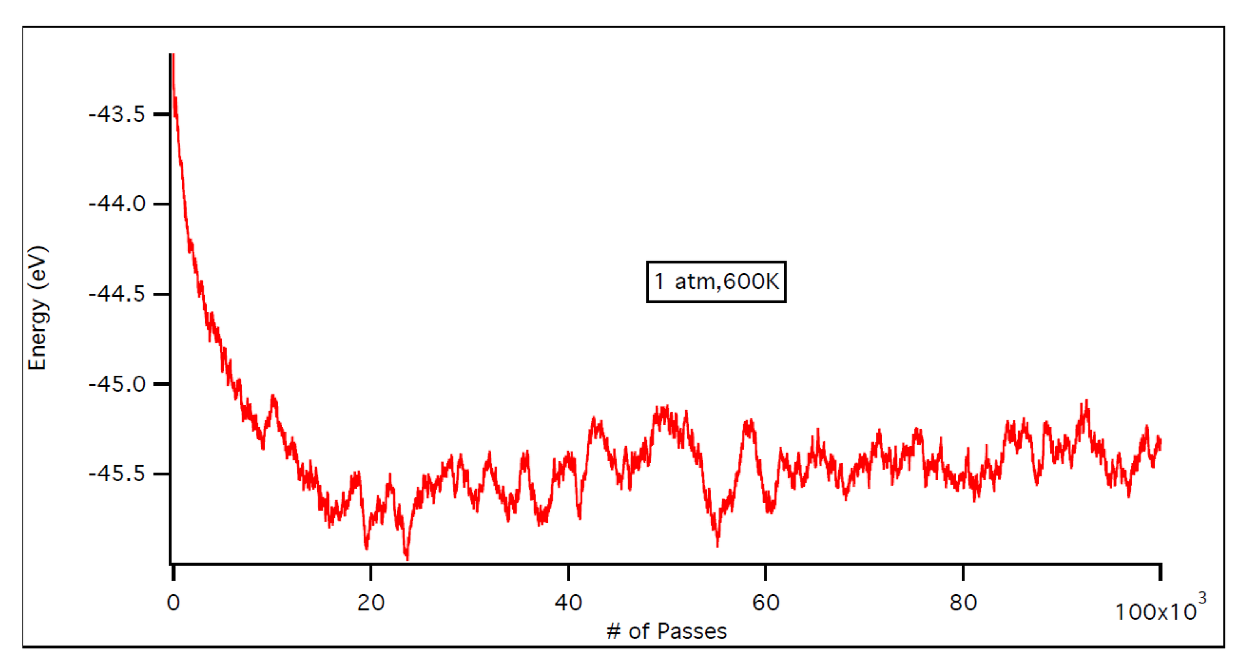
Methods and Materials

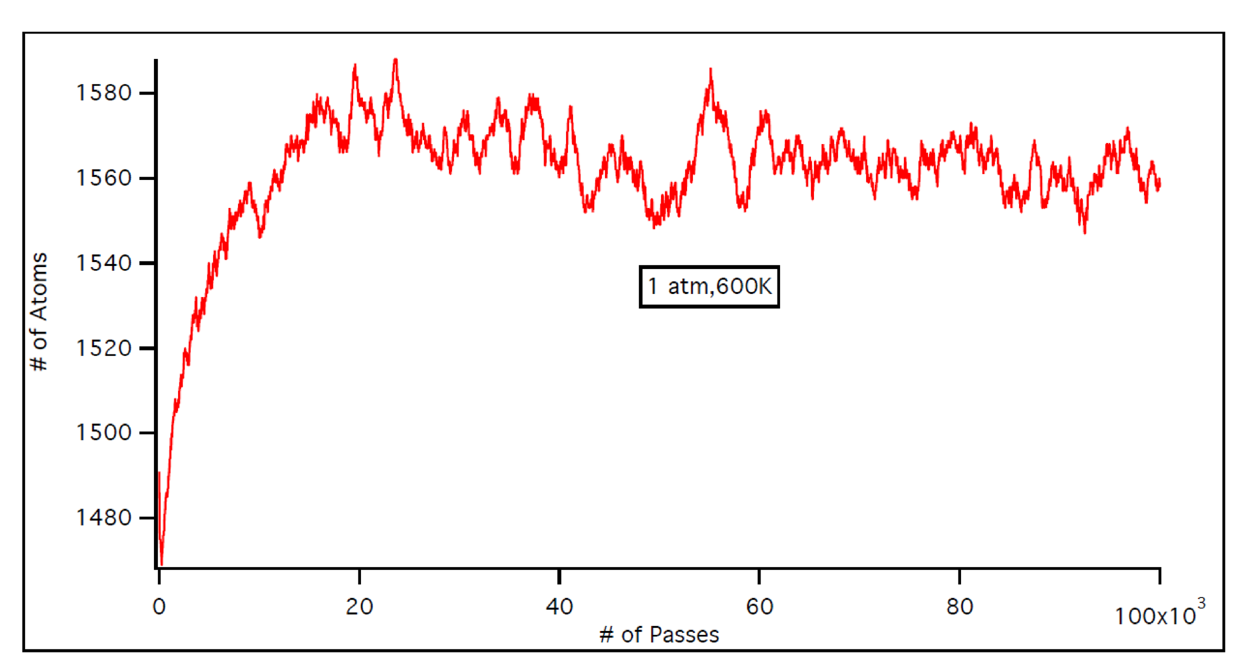
In a Monte Carlo simulation a change is first proposed to an existing system. This move is then either accepted or rejected, based on a series of probabilities calculated for that specific change. In the case of the research conducted this past summer, a Grand Canonical code was used for the simulations, meaning that the chemical potential (μ), volume (V), and temperature (T) of the system were kept constant throughout the entirety of each run. The following equation shows the embedded atom force field that was used:

$$U = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} \phi_{ij}(r_{ij}) + \sum_{j=1}^{N} F_j\left[\sum_{\substack{i=1\\ i\neq j}}^{N} \rho_{ij}(r_{ij})\right]$$

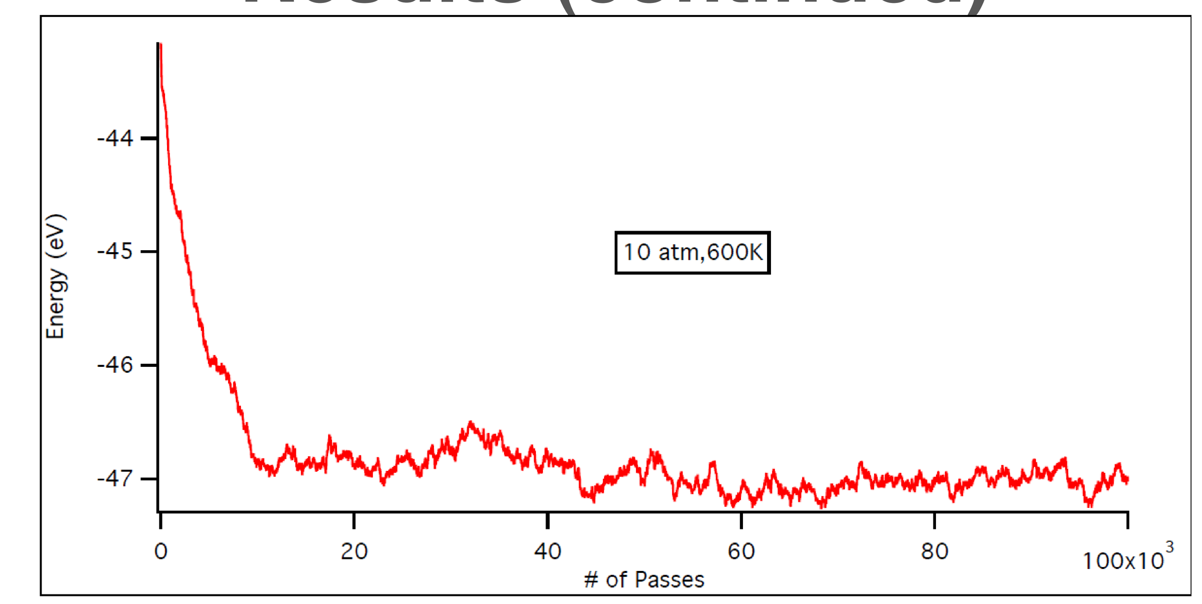
Results

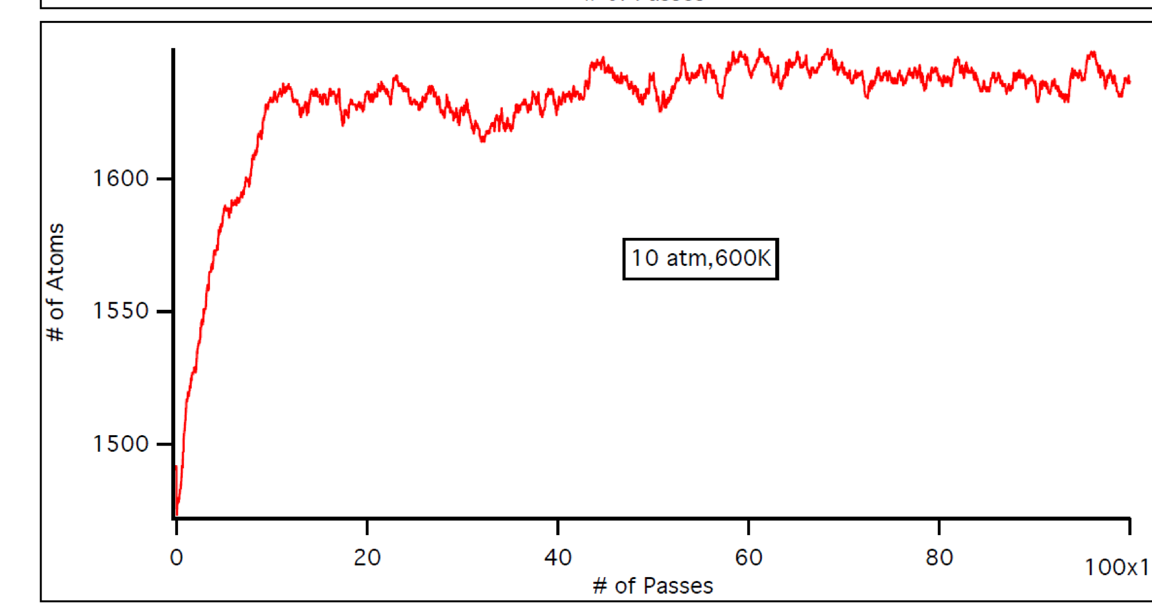


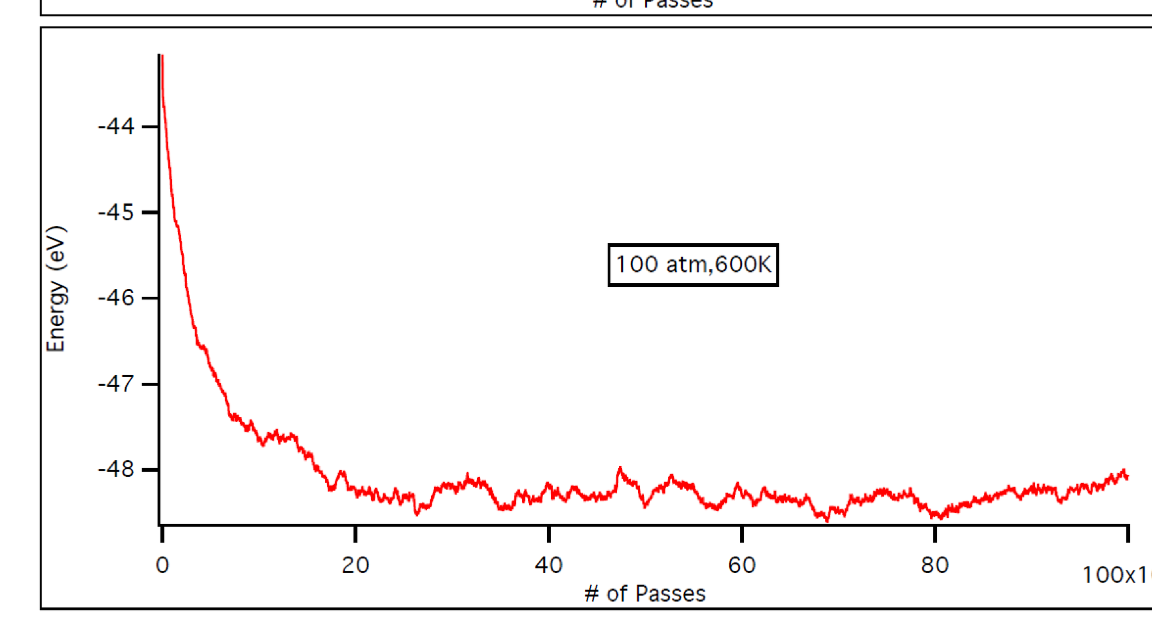


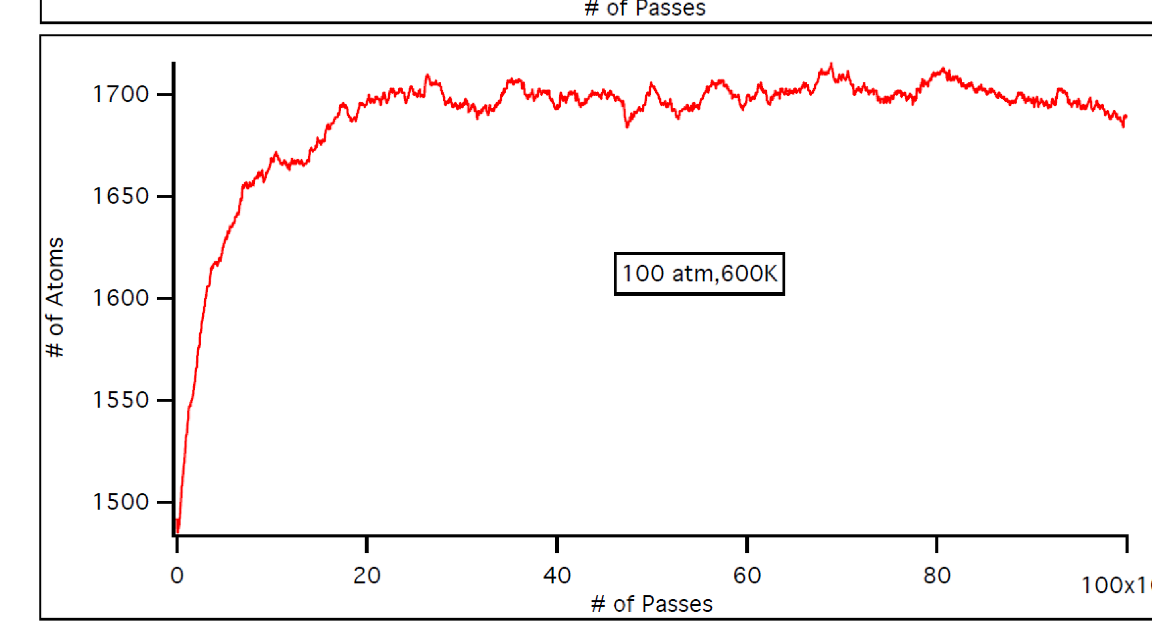


Results (continued)









As can be seen from these graphs, when the pressure of the system is increased, the number of hydrogen atoms that enter into the alloy also increases. Along with this, as more hydrogen atoms are added, the energy of the system should decrease, as is confirmed by the graphs.

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