Dimension	Description	Example of Deduction Points	Deduction Reference Value
Syntax Correctness	Examines whether the script follows LAMMPS syntax, avoiding command errors or typos.	Syntax errors, such as using non-existent LAMMPS commands or spelling mistakes.	1
Logical Consistency	Assesses whether the script is logically correct in terms of basic physical logic, e.g., whether the lattice structure matches the task requirements.	Simple logical errors, such as using FCC lattice structure when BCC was required.	1
Parameter Rationality	Examines whether physical parameters (e.g., potential function parameters, ensemble parameters) are scientifically reasonable.	Parameter errors, such as incorrect L-J potential parameters or wrong NPT settings.	1
Core Logic Accuracy	Assesses whether the script is correct in core physical computation processes, e.g., whether the density calculation method is accurate.	Critical computational logic errors, such as using the wrong density calculation method.	2
Logical Completeness	Assesses whether the script includes all necessary logical steps, e.g., setting up the potential function, temperature control, etc.	Missing logic, such as not setting a potential function or having no temperature control.	2
Code Completeness	Examines whether the script structure is complete, and whether it contains all the necessary logical modules to complete the simulation task.	Incomplete code, missing large sections of logic, such as only building the structure without simulating any process.	3