Mechanism of Transverse Cooling and Heating in Ion Channeling ◇

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Since the effect of transverse cooling and heating was experimentally established five years ago by our group, several tasks have been undertaken in search of a theoretical explanation. According to the standard theory of ion channeling the probabilities for channeled ions to become dechanneled is as large as for the reversed process, where non-channeled ions become channeled. This so-called rule of reversibility is strongly violated in the experiments performed by our group [1,2]. Depending on the experimental conditions an initially isotropic ion flux impinging on a single crystal is, after transmission, either strongly enhanced along crystal directions ("transverse cooling") or reduced ("transverse heating"). The term transverse cooling means that the ion's transverse momentum relative to crystal directions is reduced, such that non-channeled ions become "cooled down" into channels, whereas in case of transverse heating ions are thrown out ("heated up") of channels.

The most intriguing experimental finding was the transition from cooling to heating when the ion energy drops below a distinct transition energy [3]. While the body of data became larger and larger, leading to a quite complex behavior of the effect, a theoretical understanding seemed far away. From the very beginning it was reckoned that the underlying mechanism has something to do with charge exchange. Experiments with fully stripped ions have shown that in this case the rule of reversibility is strictly fulfilled despite the presence of energy loss, thus ruling out this prima facie source for violating reversibility. Most of our experiments took place around 1 MeV/u, that is, around the Bragg maximum of electronic energy loss. In this region any perturbation treatment of this many-body problem is invalid. However, non-perturbative purely quantum mechanical approaches are not available, if not impractical at all. Thus, only quite qualitative estimates could be developed so far [1].

This status was significantly changed by our own development of a computer simulation based upon a procedure known as Classical Trajectory Monte-Carlo (CTMC). Within CTMC the system under study is treated as consisting of point particles interacting via Coulomb forces/potentials and the initial conditions taken from quantum mechanics [4]. Up to now such "n-body CTMC" (n-CTMC) procedures were exclusively set up for *single* ion-atom collisions. However, in order to simulate ion channeling a many-atom type of CTMC had to be developed, now called nN-CTMC, whereby the ion interacts *simultaneously* with N crystal atoms each carrying n electrons. It must be pointed out that nN-CTMC is not just a trivial scaling from n-CTMC (with $N = 1$), as it requires several new concepts [5].

With the help of nN-CTMC it is for the first time possible to calculate the impact parameter dependence of the charge state of swift heavy ions during the oscillation between two strings of crystal atoms. The key point towards the understanding of transverse cooling and heating was the calculation of the impact parameter dependent *adiabatic* charge states, that is, those charge states which would be taken on at every impact parameter if the ion spent an infinite amount of time there. During channeling the ion stays at each accessible impact parameter only for quite a short time, such that its charge state tends indeed towards the adiabatic one, but can never reach it completely. In other words, the actual impact parameter dependent ion charge states always runs behind the goal set up by the adiabatic one.

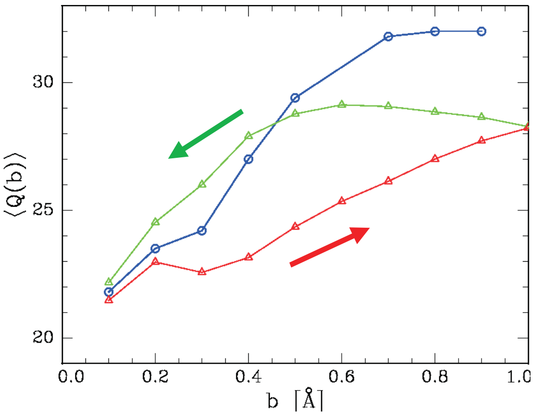

Fig. 1: Impact parameter dependent charge states in case of cooling during approaching and leaving the lattice string at $b = 0.0$ (triangles) compared with adiabatic ones (circles). A hysteresis behavior tending towards the adiabatic states is seen.

As is shown in Fig. 1, there is a difference of this running behind between the ion approaching a crystal string as compared to leaving the string. Consequently, we have discovered a "hysteresis" behavior, leading to a time dependence in the transverse channeling potential, and therefore, finally to the violation of reversibility: if, as displayed in the Figure, the ion charge state is higher while approaching the string than when leaving it, the ion-string potential is smaller on the leaving part, hence the ion has lost transverse energy/momentum, thus transverse cooling occurred. It was found that in case of heating the hysteresis behavior is just reversed.

This reversal occurs quite close at the observed transition energy from cooling to heating. At this point the electron capture probability becomes nearly independent from the impact parameter, thus the ion charge state is then determined mostly by electron loss which is weaker in the middle of the channel than when moving close to a string. Therefore, the ion charge state is then higher at small impact parameters and small in the channel middle, which is the opposite situation as shown in Fig. 1 in case of cooling.

References

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