Eur. Phys. J. D **41**, 275–279 (2007)
DOI: 10.1140/epjd/e2006-00217-9

THE EUROPEAN PHYSICAL JOURNAL D

Charge exchange collisions of H^+/D^+ ions with alkaline Earth atoms (Ca, Mg)

M.K. Pandey, R.K. Dubey, and D.N. Tripathi[a]

Department of Physics, Banaras Hindu University, Varanasi-221 005, India

Received 24 March 2006 / Received in final form 24 June 2006
Published online 27 September 2006 –

Abstract. The Classical Trajectory Monte Carlo (CTMC) Method has been used to calculate the differential, partial and total single electron capture cross sections for the collision of H^+/D^+ with Ca and Mg atoms in the energy range of 1–100 keV. The differential cross sections at angles near the diffraction limit ($<0.1^\circ$) in both systems show a forward peak followed by an asymptotic fall at higher angles. Total and partial capture cross sections are found to be in good agreement with the experimental observations. Oscillations in the partial capture cross sections have been explained due to the swapping of the field electron. Isotope effect in the electron transfer is reported to be negligible.

PACS. 34.70.+e Charge transfer – 34.10.+x General theories and models of atomic and molecular collisions and interactions (including statistical theories, transition state, stochastic and trajectory models, etc.)

1 Introduction

The investigation of charge transfer between hydrogen ions and metal atoms having two valance electrons is interesting for several reasons. Such collisions have remained a challenging task for other existing theoretical treatments and are also, relevant for several astrophysical applications. Charge transfer collisions between hydrogen ions and metal atoms in vapour phase have been investigated by several groups [1–11]. For example, the absolute capture cross sections for H^+/D^+ + Ca collisions in the energy range of 1 keV to 30 keV have been measured by Mayo et al. [12], which are in reasonable agreement with the results obtained from the classical binary encounter approximation. Tabata and Ito [13] derived an analytic formula for the single electron capture cross section using a least square fit to the experimental data of Mayo et al. [12]. Total electron capture cross section in case of H^+ colliding with Mg atom have been measured by several groups of workers for example, by II'in et al. [1] in the energy range of 10 to 150 keV, by Futch and Moses [2] in the energy range 4–50 keV, by Berkner et al. [3] in the energy range 5–70 keV, by Morgan and Eriksen [4] in the energy range 1–100 keV, by Cisneros et al. [11] in the energy range 1–5 keV, by DuBois [8] and by DuBois and Toburen [7] in the energy range 2–100 keV and by Shah et al. [10] in the energy range 90–500 keV. Calculations have been carried out on this system by several groups using the three state close coupling [6], Classical Trajectory Monte Carlo [6], classical binary encounter approximation [5] and the impact parameter formalism [9]. A close-coupling calculation based on expansion of the wave function in terms of the atomic-orbitals on the two collision centers for the system $H^+ + Mg(2p)$ has been done by Chen and Lin [14]. Total and partial cross sections have also been calculated by Amaya-Tapia et al. [15] in the energy range 1–500 keV using the semi-classical impact parameter method with a two-centre atomic basis expansion. The differential cross sections however, have so far neither been measured nor calculated for any of the two systems for which results are reported in the present investigation.

The success of the CTMC method in studies of collisions of ions with single valence electron atoms, in particular Rydberg atoms [16], in predicting the ionization and capture cross sections at intermediate energies has prompted us to apply it to other atoms. In the present work therefore, CTMC method has been used with Coulomb like interaction potential to determine the differential, partial and total single electron capture cross sections for H^+/D^+ collisions with Ca and Mg atoms in the incident energy range of 1 to 100 keV. The good agreement between the presently calculated total and partial capture cross sections with the previous results is taken as an evidence for the reliability of the reported differential cross sections. The good agreement between the present CTMC cross sections with the experimental results suggests that with a plausible interaction potential it can well simulate the differential as well as the total capture cross section

[a] e-mail: dnt@bhu.ac.in, dnt_bhu@yahoo.co.in

Table 1. Potential parameter [15,26].

	Z_0	Z_1	Z_2	Z_3
Ca	1.0	−19.0	−15.0	2.363
Mg	1.0	−11.0	−1.9	2.1

in case of collisions of proton/deuteron with two valence electron atoms.

2 Theory

The CTMC simulation of ion-atom collisions is a non-perturbative method which is well described by Abrines and Percival [17,18] and has been used by several workers [19–22]. It explicitly includes all the three body three-dimensional effects. Also, the quantal nature of the collision system, to some extent, is taken care of in the characterization of the initial state of the interacting electron.

In the present work the interaction potential used to describe the interaction between target ionic core and the remaining electron (e^-+ Ca^+ and Mg^+) is written as,

$$V(r) = -\frac{Z_0}{r} + \frac{(Z_1 + Z_2 r)}{r}\exp(-Z_3 r) \qquad (1)$$

where Z_0, Z_1, Z_2, and Z_3 are the parameters and r is the distance between the electron and the target core. The parameters given in Table 1, are chosen to give a correct asymptotic behaviour of the potential at large and small values of r.

The core-core interaction is however, taken to be a pure Coulomb one. Hamilton's equation for this three body (projectile + target + field electron) system is solved numerically using the above interaction potential in three dimensional Cartesian co-ordinates [23]. Kepler's equation has been solved to locate the electron in its orbit. The $|n\rangle$ state is specified by the binding energy E_0 and the following five pseudo-random parameters: the eccentricity ε of the Kepler orbit, the three Euler angles ϕ, ψ, θ fixing the plane of the orbit in space, and the eccentric angle u fixing the initial position of the electron on the orbit [these parameters are distributed in the following ranges [23]: $\varepsilon^2 \in (0,1)$, $\phi \in (-\pi, +\pi)$, $\Psi \in (-\pi, +\pi)$, $\cos\theta \in (-1, +1)$, $u \in (0, +2\pi)$]. Several hundred thousand trajectories are computed to determine the probability and therefore the cross section for a single electron capture.

Cartesian coordinates (which are known all through the collision time) of the colliding partners after the collision have been used to determine the centre of mass scattering angle. The angular differential cross sections for the single electron capture were computed using the formula,

$$\frac{d\sigma_{cap}}{d\Omega} = \frac{2\pi\, b_{\max} \sum_j b_j^{(i)}}{N \Delta\Omega}, \qquad (2)$$

and the standard deviation for the cross section is given by

$$\Delta\sigma_{cap} = \sigma_{cap}\left(\frac{N - N_{cap}}{N N_{cap}}\right)^{1/2}. \qquad (3)$$

N is the total number of trajectories calculated for an impact parameter less than $b_{\max}$, N_{cap} is the number of trajectories that satisfy the criteria for capture, $b_j^{(i)}$ is the impact parameter for which the criteria for capture is fulfilled and $\Delta\Omega$ is the emission solid angle interval of the captured electron. The statistical error limit to a good approximation can be written as $\Delta\sigma \approx \sigma/N_{cap}^{1/2}$. This implies that in order to reduce the error in the calculation one has to take a large number of trajectories. For the results presented here more than 10^5 trajectories were computed to obtain good statistics (<3%) for the differential cross section.

Estimation of the n, l distribution of the final state after electron capture has been done as follows [16]: the energy of the captured electron relative to the projectile (E_{ep}) is used to obtain a classical principal quantum number n_c. This number is further quantized to a level specified by the quantum number n. The normalization of the classical angular momentum l_c yields an orbital angular momentum quantum number l. Once the capture state is specified with its n and l quantum numbers, the probability of capture in it is calculated.

The one-electron probabilities have been used in the evaluation of the independent-particle multielectron probabilies [24]. Given a capture probability to be P for the first electron transfer, the probability for the 2nd electron to be transferred is $(1-P)P$. Following this procedure the total probability for the one electron to be transferred out of N equivalent electrons becomes $1-(1-P)^N$. In the present case with two electrons in the s-orbital therefore, it is given by $1-(1-P)^2$.

3 Results and discussion

Differential cross sections for single electron capture to all the states are calculated at different incident energies and the results for angles close to the diffraction limit for Ca as well as Mg atoms are shown in Figures 1 and 2, respectively. This is because the typical scattering angles of interest are only a fraction of a degree (<0.1°) for projectile energies in the keV range in which the scattering amplitudes (and hence the differential cross sections) for the various reaction channels are expressed as a Fraunhofer type integral [25]. In the present case however, the Fraunhofer type of diffraction pattern due to annular ring, well-known in classical optics, does not appear. The reason may be the presence of the two electrons in the valence shell. Instead their magnitude (at all the energies) peaks in the forward direction and decreases asymptotically with an increase in the scattering angle. It is also noted that the differential cross section in the forward direction is maximum at the projectile energy of 5 keV followed by 10 and 1 keV of energies, respectively. The nature of the variation of the differential cross section with angle in case of Mg atom is similar to that of the Ca atom. At 1 keV of incident energy the charge transfer cross sections to 1s state of hydrogen atom are also shown for both the targets viz; Ca and Mg in Figures 3 and 4, respectively.

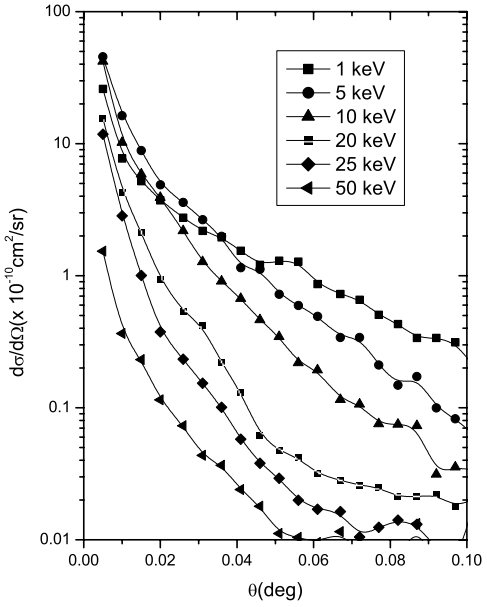

Fig. 1. Differential cross sections for single electron capture to all states at incident energies of 1, 5, 10, 20, 25, and 50 keV for H^+ + Ca collision.

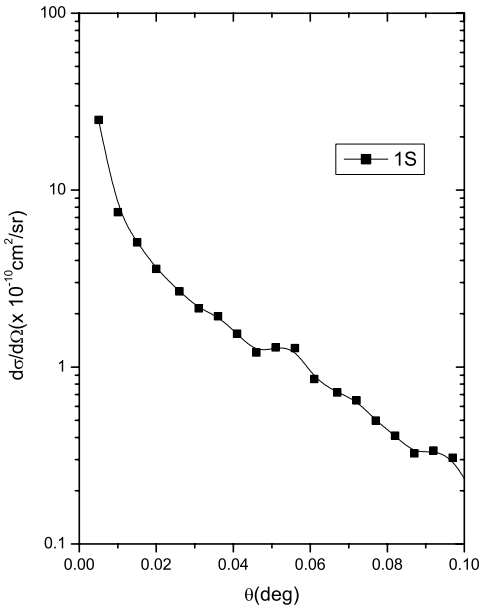

Fig. 3. Differential cross sections for single electron capture to 1*s* states at incident energies of 1 keV for H^+ + Ca collision.

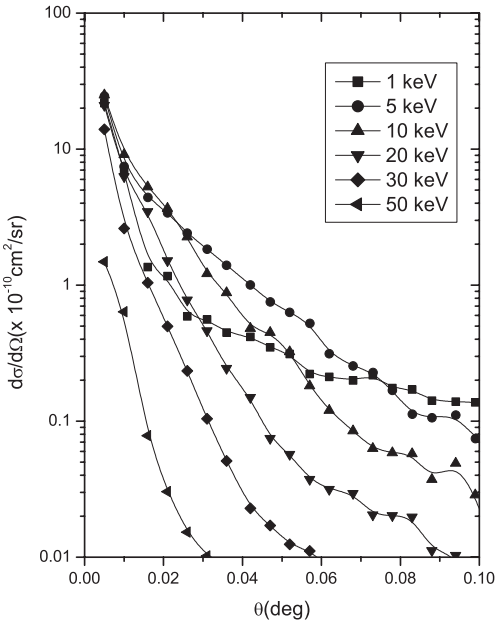

Fig. 2. Differential cross sections for single electron capture to all states at incident energies of 1, 5, 10, 20, 30 and 50 keV for H^+ + Mg collision.

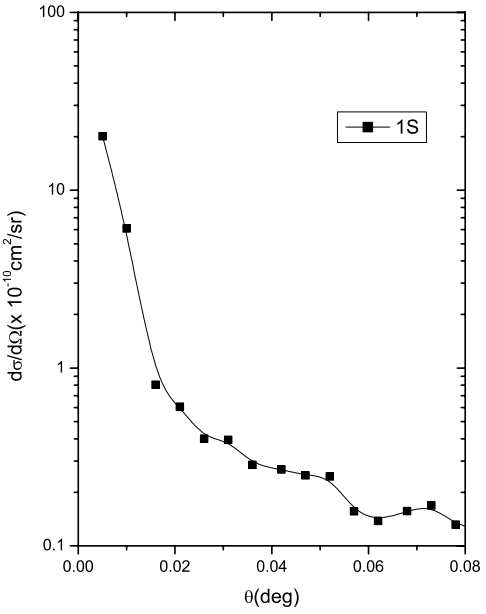

Fig. 4. Differential cross sections for single electron capture to 1*s* states at incident energies of 1 keV for H^+ + Mg collision.

In both the cases the nature of the variation of the cross sections with energy is similar.

The total cross sections for single electron capture for Ca atom are shown in Figure 5. The present results are in very good agreement with various experimental [12] as well as theoretical [12,26] results. CTMC results have reproduced not only the shape but also the magnitude of the observed data of Mayo et al. [12] as well as the semiclassical impact parameter calculations of Martínez et al. [26] in the entire energy range. It is noticed that the variation of the total capture cross section with energy conforms to that of the differential cross section which after increasing up to 5 keV decreases. In order to see the isotope effect, all the above mentioned capture cross sections for the deuteron projectile have been calculated but the results are given only for the total cross sections (see Fig. 6). Capture cross section with deuteron as projectile remain similar to the proton indicating thereby, an absence of the isotope effect.

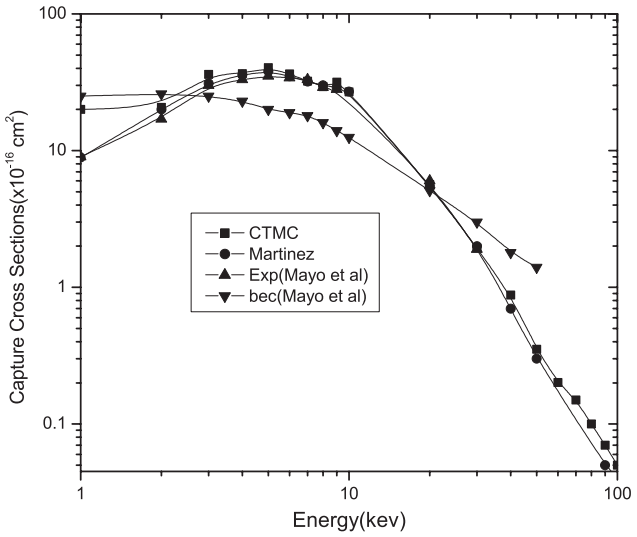

Fig. 5. Total capture cross sections for the H^+ + Ca collision.

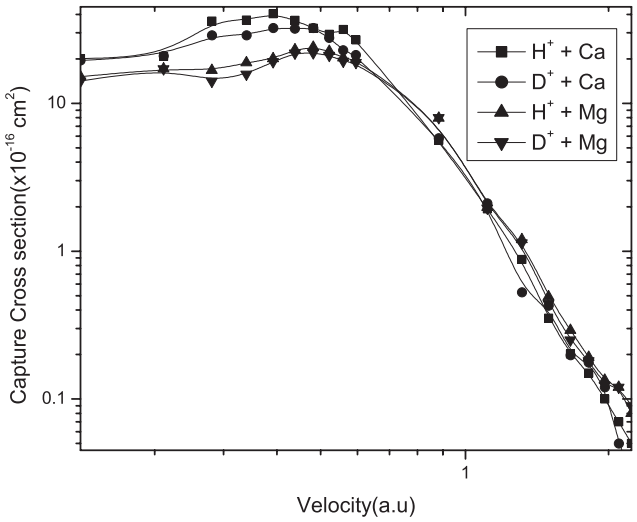

Fig. 6. Total capture cross sections for the H^+/D^+ + Ca and Mg collision at different projectile velocity.

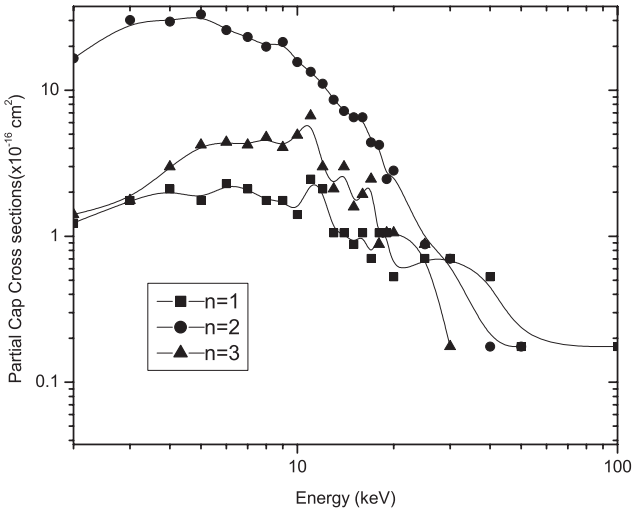

Fig. 7. Partial capture cross sections for the H^+ + Ca collision.

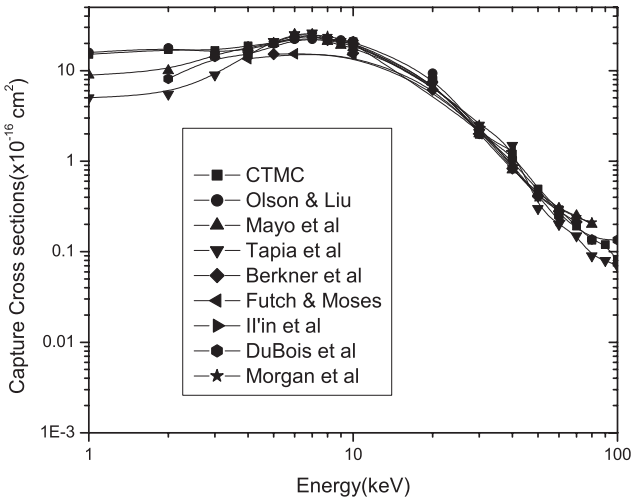

Fig. 8. Total capture cross sections for the H^+ + Mg collision.

The calculated results of partial capture cross sections for $n = 1$, 2, and 3 shells of hydrogen atom are given in Figure 7. At lower impact energies it is the energy defect ΔE (the energy difference between the initial and final states of the captured electron) that primarily governs the process of capture. Accordingly, it can be seen from Figure 7 that the capture cross section to the $n = 2$ level is maximum up to 25 keV. Further, below this energy the relative magnitudes of the partial cross sections corresponding to $n = 2$, 3 and 1 levels are ordered according to their respective energy defects viz 0.0997, 0.1691 and 0.275 au. The present result is in good agreement with the findings of Martínez et al. [26]. In case the collision velocity is smaller than orbital velocity of the electron in an atom, for the ion-atom interaction the potential surface, which determines the electronic dynamics, is characterized by a saddle between the projectile and the target. At some critical internuclear separation the electron becomes free to travel back and forth between the target and projectile centres. The oscillations associated with the swapping (or crossing of the saddle) of the electronic density are well-known [22,27] to exist where the number of swaps that the electron undergoes are correlated to the structure in the capture cross section. The oscillations appearing in the reported partial cross sections, shown in Figure 7, are the manifestation of this effect. These structures provide a novel measure of the time dependent beating of the non-stationary molecular wave packet which is formed at the moment over-barrier transitions become classically allowed. These oscillations disappear in the total capture cross sections due to the averaging.

The results for single electron capture cross sections for H^+ + Mg are shown in Figure 8. The calculated cross sections are in very good agreement with the available theoretical [6,12,15,26] as well as experimental [1–3,7,26] results in the entire energy range. The largest discrepancy is observed at energies below 3 keV where our calculated cross section is twice that of Amaya-Tapia et al. [15]. However, it is in agreement with the calculated results of Olson

and Liu [6]. The maximum value of the capture cross section is obtained at 7 keV of incident energy after which it decreases rapidly. Differential as well as total capture cross sections with deuteron as the projectile have also been calculated. The result as in case of Ca however, is given only for the total cross sections (see Fig. 6). It remains more or less the same as that with proton as the projectile. This further confirms an absence of isotope effect in electron capture from two valence electron target atoms [5].

4 Conclusions

It has been shown that CTMC method for the calculations of the charge transfer cross section for H^+/D^+in collision with atoms having two valance electrons (Ca, Mg) like that of single valence electron atom is an acceptable method. Oscillations in the partial capture cross sections have been explained due to swapping of the field electron. Isotope effect in the electron transfer is reported to be negligible.

The authors are grateful to Prof. D.K. Rai for his valuable help in its discussion part and Dr B. Singh (Dept. of Physics, Udai Pratap Post Graduate College, Varanasi) for the encouragement and support during the course of this work. One of the authors Ritesh Kumar Dubey thanks the Council of Scientific and Industrial Research (CSIR), Govt. of India, New Delhi for financial support.

References

1. R.N. II'in, V.A. Oparin, E.S. Solov'ev, N.V. Fedorenko, Sov. Phys-JETP Lett. **2**, 197 (1965)
2. A.H. Futch Jr, K.G. Moses, *5th Int. Conf. on Physics of Electronic and Atomic Collisions*, edited by I.P. Flaks, E.S. Solov'ev (Nauka, Leningrad, 1967), Abstracts of papers, p. 12
3. K.H. Berkner, R.V. Pyle, J.W. Stearns, Phys. Rev. **178**, 248 (1969)
4. T.J. Morgan, F.J. Eriksen, Phys. Rev. A **19**, 1448 (1979)
5. T.J. Morgan, F.J. Eriksen, Phys. Rev. A **19**, 2185 (1979)
6. R.E. Olson, B. Liu, Phys. Rev. A **20**, 1366 (1979)
7. R.D. DuBois, L.H. Toburen, Phys. Rev. A **31**, 3603 (1985)
8. R.D. DuBois, Phys. Rev. A **34**, 2738 (1986)
9. J.C. Garcia-Madroñal, O. Mo, *Proc. 17th Int. Conf. on Physics of Electronic and Atomic Collisions*, Brisbane, Australia, edited by I.E. McCarthy, W.R. Gillivray, M.C. Standange (Adam Hilger, Bristol, 1991), p. 403
10. M.B. Shah , P. McCallion, Y. Itoh, H.B. Gilbody, J. Phys. B: At. Mol. Opt. Phys. **25**, 3693 (1992)
11. C. Cisneros, H. Martínez, B.E. Fuentes, I. Alvarez, J. de Urquijo, I. Dominguez, Nucl. Instrum. Meth. B **117**, 1 (1996)
12. M. Mayo, J.A. stone, T.J. Morgan, Phys. Rev. A **28**, 1315 (1983)
13. T. Tabta, R. Ito, Nucl. Instrum. Meth. Phys. Res. B **31**, 375 (1988)
14. Z. Chen, C.D. Lin, Phys. Lett. A **194**, 201 (1994)
15. A. Amaya-Tapia, R. Hernández-Lamoneda, H. Martínez, J. Phys. B: At. Mol. Opt. Phys. **34**, 769 (2001)
16. A.N. Perumal, D.N. Tripathi, Nucl. Instrum. Meth. B **143**, 429 (1998)
17. R. Abrines, I.C. Percival, Proc. Phys. Soc. **88**, 861 (1966)
18. R. Abrines, I.C. Percival, Proc. Phys. Soc. **88**, 873 (1966)
19. R.E. Olson, A. Salop, Phys. Rev. A. **16**, 531 (1977)
20. G. Peach, S.L. Willis, M.R.C. McDowell, J. Phys. B: At. Mol. Opt. Phys. **18**, 3921 (1985)
21. J. Pascale, R.E. Olson, C.O. Reinhold, Phys. Rev. A **42**, 5305 (1990)
22. A.N. Perumal, D.N. Tripathi, Phys. Rev. A **64**, 042709 (2001)
23. A.N. Perumal, Ph.D. thesis, Dept. of Physics, B.H.U. India, 1998
24. B. Hamre, J.P. Hansen, L. Kocbach, J. Phys B: At Mol. Opt. Phys. **32**, L127 (1999)
25. L. Wilets, S.J. Wallace, Phys. Rev. **169**, 84 (1968)
26. H. Martínez, A. Amaya-Tapia, J. Phys B: At Mol. Opt. Phys. **36**, 3509 (2003)
27. K.B. MacAdam, J.C. Day, J.C. Aguilar, D.M. Homan, A.D. MacKellar, M.J. Cavagnero, Phys. Rev. Lett. **75**, 1723 (1997)